DTU Chemical Engineering

Annual Report 2011

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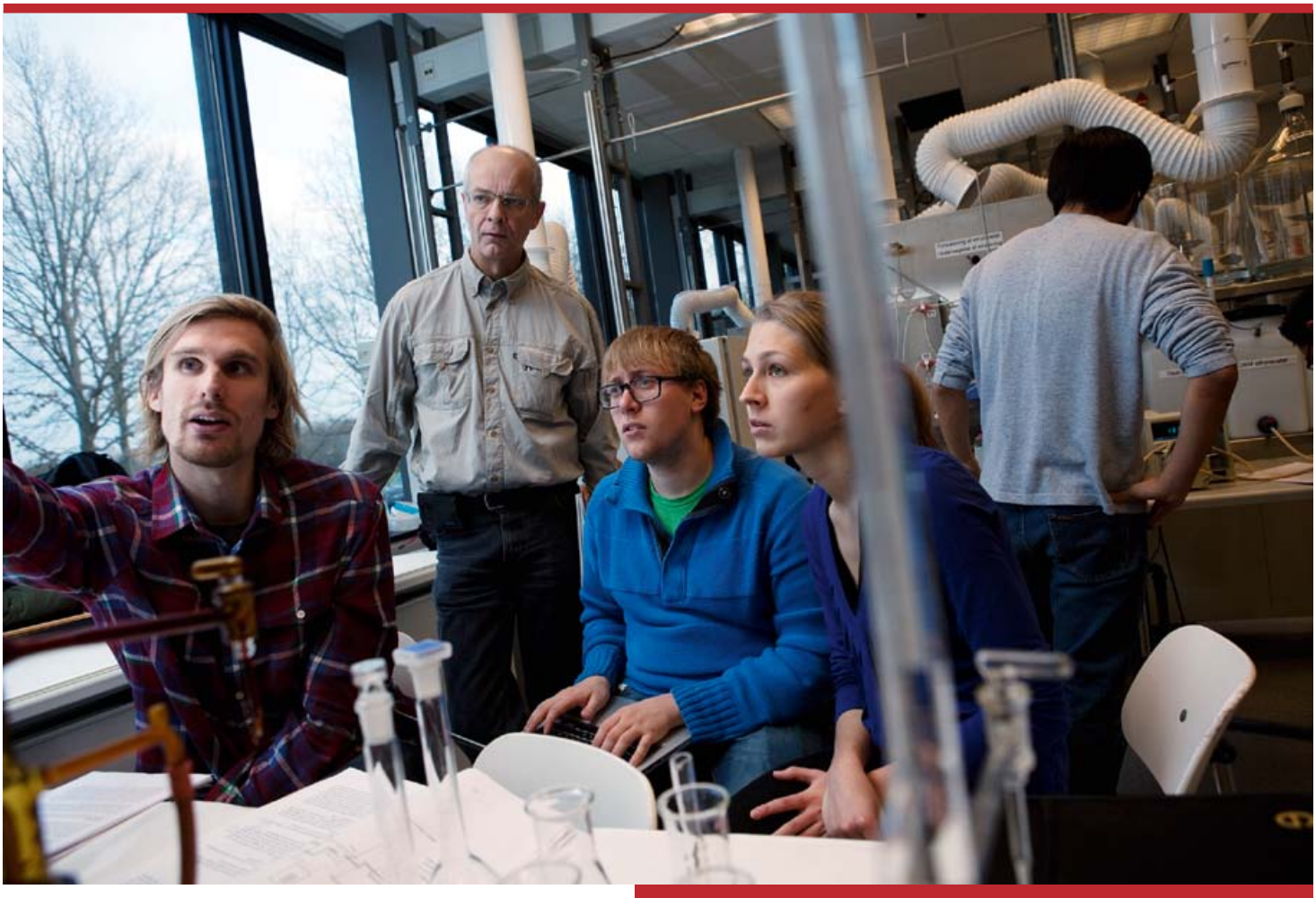

DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

Annual Report 2011
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ANNUAL REVIEW

Head of Department

NEW AND EXCITING CHALLENGES

Kim Dam-Johansen
Professor, Head of Department

2011 was yet again an exciting and successful year for DTU Chemical Engineering. We consolidated existing collaboration and research activities while at the same time broke new ground in both the chemical and biochemical engineering field and disciplines.

The real strengths of our department are the strong research centers and their close interdisciplinary cooperation. AT-CERE has consolidated the interaction with other departments in the important field of Petroleum Engineering in the cross-departmental center, CERE. CHEC has continued expansion in its traditional field of high-temperature processes and emission control and developed new and expanding activities related to advanced coatings and continuous pharma production in close cooperation with other centers at the department. DPC is breaking new ground in the polymer area in large research projects with new industrial partners. CAPEC and PROCESS merged forces to further expand their international industrial consortium and fine tune and accelerate advances in the process-product areas, with experimental and theoretical process optimization and reliable and sophisticated mathematical models. And BioEng explores and expands the critical and highly applicable field of enzyme technology with an effective enzyme production platform as a working horse for new activities.

Our unwavering commitment to research is matched by our commitment to educate our students with critical knowledge and key skills to meet the demands of industry and society in a globalized world. Our student organization became still more active during the year and we continued internationalization of our educations.

Students in Focus – and in the Limelight

In 2011, our students received much recognition. Four students won the first prize in the 2011 Venture Cup, PhD student Ane Avlund was the 2011 Christopher J. Wormald prize winner, and two master students received the Novo Scholarship and Carlsberg Scholarship, respectively.

Professor Anne S. Meyer was awarded PhD supervisor of the year – recognition of students also includes excellent supervision. Graduate student, Adam Duranni, and senior researcher Ulrich Krühne participated in a live broadcast of DR2's program Deadline on the topic of 3D printing of micro fluidic systems.

2011 also welcomed back a host of international students to the increasingly popular Summer University – during the summer holidays, 56 European and American students got hands-on experience in our pilot labs.

Senior Focus

On 28 January Associate Professor Flemming Frandsen defended his doctoral thesis on 'Ash Formation, Deposition and Corrosion when Utilizing Straw for Heat and Power Production' – a gigantic effort solidly based on 15 years of excellent research.

2011 also saw a new professor as center leader of AT-CERE, Georgios Kontogeorgis, who was appointed professor in Chemical and Biochemical Thermodynamics at DTU Chemical Engineering.

Our Professor Emeritus John Villadsen was appointed honorary doctor at UAM in Mexico, while I was appointed honorary doctor at Åbo Academy, Finland, honorary professor at Institute of Process Engineering and Einstein Professor at CAS, both China.

Professor Søren Hvilsted celebrated 25 years at Risø and DTU, a period marked by excellent and very productive research.

The department could also welcome three new members of Faculty; Assistant Professors Jakob Kjøbsted Huusom, Anders Egede Daugaard and Philip Fosbøl. Anne Ladegaard Skov and Gürkan Sin were both promoted Associate Professors.

International cooperation

The department continued its expansion of international collaboration in 2011. Professor Rafiqul Gani was elected to the board of trustees of CAChE (Computer Aids for Chemical Engineering) and explored new ground with Chulalongkorn University, in Bangkok, Thailand. The Far East is increasingly coming into focus, and the department continues and expands its commitment to the Sino-Danish Center for Research and Education.

In November 2011, our management team visited the Korean Advanced Institute of Science and Technology (KAIST) to explore cooperation in the field of biorefineries. In 2012 KAIST professors are to revisit our department at DTU.

Promising future

On 1 January 2012 the previous organization, DTU Risø Biosystems, together with other activities were integrated into DTU Chemical Engineering. In one step the department expanded significantly both in capabilities, in human resources and in physical infrastructure. The department will in the future have activities at two main locations: Campus Lyngby and Campus Risø. It is our ambition and plan to face our new challenges and potential and build new working methods to stay in the absolute international elite among chemical engineering departments.

I hope you will enjoy reading our 2011 Annual Report and join us on our continued and shared path into the exciting and promising world of chemical and biochemical engineering.

Kim Dam-Johansen
Professor, Head of Department

HIGHLIGHTS 2011



1) Georgios Kontogeorgis is appointed professor, photo: Christian Carlsson. **2, 3, 4)** Science Camp students win a day at DTU Chemical

HIGHLIGHTS 2011

JANUARY

JANUARY 1

Dr. Jakob Kjøbsted Huusom employed as Assistant Professor

Jakob Kjøbsted Huusom finished both his MSc and PhD at DTU Chemical Engineering and has worked at the department in a postdoc position for the last two years. Jakob Kjøbsted Huusom has taught at University of Trinidad and Tobago under a DTU exchange program. Huusom's research interests primarily lie within dynamic modeling and simulation of chemical and biochemical processes, with a special interest in process control.

JANUARY 1

Professor Rafiqul Gani elected to the board of trustees of CAChE

Professor Rafiqul Gani is elected to the board of trustees of CAChE (Computer Aids for Chemical Engineering). CAChE is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

JANUARY 4

CAPEC-PROCESS Industrial Consortium formally established

The CAPEC and PROCESS research centers formally combine their industrial consortium activities in one industrial consortium known as CAPEC-PROCESS Industrial Consortium.

JANUARY 21

First prize to four students in 2011 Venture Cup

Four students at DTU Chemical Engineering win the first prize at the 2011 Venture Cup, hosted by a consortium of universities and leading companies in Denmark, for "the most promising idea from DTU". The idea was a result of the product development course offered by the department.

JANUARY 26

PROCESS master student receives Novo Scholarship

The PROCESS research center is for the 2nd year in a row awarded a Novo Scholarship. This year's PROCESS recipient, Hemalata Ramesh, will work on enzymatic biodiesel production for 6 months under the supervision of John Woodley, Mathias Nordblad and Yuan Xu.

JANUARY 28

Flemming Frandsen defends his doctoral thesis

Associate Professor Flemming Frandsen defends his doctoral thesis on 'Ash Formation, Deposition and Corrosion when Utilizing Straw for Heat and Power Production'. The thesis is the result of 15 years' research in the field of biomass combustion at central power plants, with a special focus on the issues related to using straw.

JANUARY 30 ①

Georgios Kontogeorgis appointed professor

Center leader of AT-CERE, Georgios Kontogeorgis is appointed professor in Chemical and Biochemical Thermodynamics at DTU Chemical Engineering. Georgios Kontogeorgis finished his MSc in chemical engineering at the Technical University

Engineering. **5)** Professor Emeritus John Villadsen appointed honorary doctor.

of Athens, Greece and completed his PhD at DTU Chemical Engineering. In the years 1997-2011 he has worked as Associate Professor and later Docent at the department.

FEBRUARY

FEBRUARY 1

Anders Egede Daugaard employed as Assistant Professor at the department

Anders Egede Daugaard finished his MSc in chemical engineering at DTU and performed his PhD work at DTU Chemical Engineering. Daugaard's primary focus area has been the development of functional materials through polymer synthesis. At University of California Santa Barbara, Daugaard has worked with dendrimer synthesis on development of new materials for holographic data storage.

FEBRUARY 2-3 ②③④

Science Camp students win a day at DTU Chemical Engineering

10 high school students, winners in Science Camp 2011 hosted by Momentum and Hillerød HTX, visit the pilot plant at DTU Chemical Engineering and get the chance to try out theory in near to real-life scale and conditions at the department's well equipped pilot plant.

FEBRUARY 10 ⑤

Professor Emeritus John Villadsen appointed honorary doctor

Professor Emeritus John Villadsen appointed honorary doctor at Universidad Autónoma Metropolitana (UAM) in Mexico. AUM states that its recommendation for the appointment of John Villadsen is based on his excellent work within the science of chemical engineering and his effort to use results of this research on biological systems for the benefit of the development of the biotechnological industry.

APRIL

APRIL 27-30

Professor John Woodley teaches at PhD summer school in Italy

The PhD summer school 'Multi-step cascade biocatalysis' is organized by COST in Siena, Italy.

MAY

MAY 5

Model Based Control Conference at DTU co-organized by CAPEC

125 people attend the conference with Prof. James B. Rawlings as keynote speaker. Prof. Rawlings is well-known for his contributions to Model Predictive Control and has had a long and lasting cooperation with the department. Prof. Rawlings was appointed honorary doctor at DTU on 6 May 2011.

MAY 15

***Permanent Plug* project initiated in Qatar**

The project, headed by Associate Professor Anne Ladegaard Skov, will study the shut-off of fractures in oil wells by use of elastomers and is funded by Maersk Oil and Gas Research and Technology Centre Qatar.



6) Karsten H. Reichstein is employed as Deputy Director at the department. Karsten H. Reichstein comes from a job as CIO at Copenhagen University Hospital (Rigshospitalet)**. 7, 8, 9)** Summer University at DTU Chemical Engineering.

HIGHLIGHTS 2011

MAY 16

Associate Professor Anne Ladegaard Skov in large DEAP research project

Highly efficient low cost energy generation and actuation using disruptive DEAP technology. The technology platform is funded for a 4-year period by the Danish National Advanced Technology Foundation and represents 3 universities and 6 companies (Danfoss Polypower A/S, ESS Technology A/S, Polyteknik A/S, Wavestar A/S, Bang og Olufsen A/S and Danfoss A/S).

MAY 20

Professor, Head of Department, Kim Dam-Johansen appointed honorary doctor

Professor, Head of Department, Kim Dam-Johansen is appointed honorary doctor at Åbo Academy University, Finland, for his research in clean and efficient combustion and for his work for the Nordic co-operation in research and education.

JUNE

JUNE 7-9

CAPEC-PROCESS Industrial Consortium Annual Meeting

The first joint CAPEC-PROCESS Industrial Consortium Annual Meeting 2011 has 93 participants, out of which 28 are member company representatives, 9 are invited guests and the rest are from CAPEC and the department.

JUNE 8-10

CERE Discussion Meeting 2011

99 people participate in the discussion meeting – and with 35 external participants representing 20 companies from 13 countries, the meeting sets a new record in industry participation. Sinopec from China, industrial consortium member since 2009, takes part with five representatives showing keen interest in carbon capture and storage (CCS).

JULY

JULY 1 ⑥

Karsten H. Reichstein is employed as Deputy Director at the department.

Karsten H. Reichstein comes from a job as CIO at Copenhagen University Hospital (Rigshospitalet).

JULY 1-30 ⑦⑧⑨

DTU Summer University 2011

56 university students from the USA and Europe participate in the Chemical & Biochemical Unit Operations Laboratory course giving them hands-on experience with large scale unit operations.

JULY 5

Professor, Head of Department, Kim Dam-Johansen appointed Einstein Professor

Professor, Head of Department, Kim Dam-Johansen is appointed Einstein Professor by the Chinese Academy of Sciences, and honorary professor at the Institute of Process Engineering, CAS. In this connection, Prof. Dam-Johansen also takes part in a Hempel Innovation workshop at which he presents the cooperation between Hempel and DTU Chemical Engineering.



10) 2011 Christopher J. Wormald prize winner. **11)** CHEC Annual Meeting 2011.

AUGUST

AUGUST 15

Bioraffinaderi Øresund, Danish-Swedish collaborative project on biorefining

A collaborative project between three DTU departments, including the PROCESS center at DTU Chemical Engineering (Dr Pär Tufvesson) and three Swedish university institutions aiming to develop biorefineries in the Øresund region is established.

AUGUST 22-25

Professor John Woodley teaches at PhD summer school in Germany

The summer school 'Biotransformations' is organized by DECHEMA at Bad Herrenalb, Germany.

AUGUST 8-19

Advanced summer school within thermodynamics

Professors Michael L. Michelsen and Georgios Kontogeorgis hold the "Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects" with 26 participants.

AUGUST 31 ⑩

2011 Christopher J. Wormald prize winner

The 2011 Christopher J. Wormald prize is presented to a PhD student in the department, Ane Avlund, during the Thermodynamics 2011 conference in Athens, for her innovative research in thermodynamics.

SEPTEMBER

SEPTEMBER 14

Professor Peter Glarborg gives plenary lecture at 7th Mediterranean Combustion Symposium (MCS7)

Professor Glarborg's lecture is on *Bio-dust Combustion for Heat and Power Production.*

SEPTEMBER 25-29

Invited keynote lecture by Prof. John Woodley and PhD student Yuan Xu

Prof. John Woodley and PhD student Yuan Xu jointly give an invited keynote lecture at the 1st European Congress of Applied Biotechnology, Berlin, Germany.

SEPTEMBER 27 - OCTOBER 7

Visit to PPC, Chulalongkorn University, Bangkok, Thailand

Professor Rafiqul Gani gives an MSc level course at The Petroleum and Petrochemical College (PPC), Chulalongkorn University, Bangkok, Thailand attended by 29 students. During his visit to PPC, Prof. Gani also discusses research collaboration in the area of sustainable chemical and bio-process design with faculty members of PPC and representatives of SCG, a member company of the CAPEC-PROCESS consortium.



12) Students with Professor James Rawlings who was awarded an honorary doctorate from DTU in 2011. **13, 14, 15**) Open House event in connection with the International Year of Chemistry 2011, photos: Christian Carlsson.

HIGHLIGHTS 2011

OCTOBER

OCTOBER 11 ⑪

CHEC Annual Meeting 2011

Around 100 participants, with many participants from leading companies in the industry, take part in CHEC's annual meeting, "Refining and Thermal Conversion of Biomass and Waste". Areas covered are *catalytic processes, thermal conversion of biomass, ashes and trace elements and industrial processes.*

OCTOBER 16 ⑫

Students take part in the AIChE Annual Meeting in Minneapolis, Minnesota

Seven students from the department present projects in a poster session at the AIChE Annual Meeting. In November 2010, the student organization at DTU Chemical Engineering was the first in Europe to get a student chapter with the AIChE.

OCTOBER 18 ⑬⑭⑮

Celebration of International Year of Chemistry 2011

Employees and students at DTU Chemical Engineering co-organize an Open House event, ÅBENT KEMIHUS, with around 80 visitors, ranging from young children to grandparents interested in science and chemical and biochemical engineering.

OCTOBER 28

Professor Anne S. Meyer appointed PhD supervisor of the year

Prof. Meyer, center leader of BioProcess Engineering at the department, is appointed PhD supervisor of the year.

OCTOBER 31

Juan de Pablo meets with faculty and PhDs at DTU Chemical Engineering

In connection with his H.C. Ørsted Lecture at DTU, Professor Juan de Pablo meets with faculty and PhD students at DTU Chemical Engineering.

NOVEMBER

NOVEMBER 1-6 ⑯

Management team visits KAIST in South Korea

The management team of DTU Chemical Engineering visits the Korean Advanced Institute of Science and Technology (KAIST) to explore cooperation in the field of biorefineries.

NOVEMBER 2

DTU Chemical Engineering featuring on national television

On Wednesday 2 November 2011, senior researcher Ulrich Krühne and graduate student Adam Duranni from DTU Chemical Engineering are participating in a live broadcast of DR2's program *Deadline.* Krühne and Duranni have been working with 3D printing of micro fluidic systems with a so-called Makerbot, a 3D printer, which comes as a self-assembly kit, taking up no more space than a tabletop.

NOVEMBER 2-3

PetroChallenge 2011 with record participation

Over 1200 high school students take part in this year's PetroChallenge, an online competition about finding oil, organized by CERE. The event was sponsored by Maersk Oil.




16) Management visit to KAIST in November. **17**) Professor Søren Hvilsted celebrates 25 years at Risø and DTU, photo: Christian Carlsson.
18) Morten Østergaard, Minister for Science, Innovation and Higher Education presents Carlsberg Scholarship to Louise With Sengeløv, photo: US Photo.

NOVEMBER 16

Risø Biosystems to be integrated into DTU Chemical Engineering

On 16 November it is announced that Risø Biosystems should be integrated into DTU Chemical Engineering as of 1 January 2012. This integration brings the total number of employees close to 300 and gives great promises for future research synergies.

NOVEMBER 18 ⑰

Professor Søren Hvilsted celebrates 25 years at Risø and DTU

Professor Hvilsted of the Danish Polymer Centre at DTU Chemical Engineering could celebrate his 25 years at Risø and DTU, a period with a very high research production.

NOVEMBER 22-24

Professor John Woodley gives a PhD course in Chile

Professor John Woodley gives a PhD course and lecture on bioprocess integration at University of Antofagasta, Chile.

NOVEMBER 24 ⑱

Master student Louise With Sengeløv receives Carlsberg Scholarship

Louise receives the Carsbergs Mindelegat Scholarship of DKK 75.000 on the basis of her master's project on *HCl emissions from modern cement production processes equipped with a by-pass* – a project performed in cooperation with FLSmidth A/S as part of the CHEC research platform sponsored by the Danish National Advanced Technology Foundation.

NOVEMBER 25

Annual Polymer Day 2011

The Graduate School of Polymer Science at DTU Chemical Engineering hosts the 7th Annual Polymer Day with 50 participants.

DECEMBER

DECEMBER 1

Philip Fosbøl employed as Assistant Professor

Philip Fosbøl is employed as Assistant Professor at the department.

DECEMBER 16

Annual Christmas Meeting with future colleagues

On 16 December the department holds its annual Christmas Meeting in which the 2012 integration of Risø Biosystems is the key subject. As of 1 January DTU Chemical Engineering will comprise close to 300 employees.


CALIFORNIA

RESEARCH & INNOVATION & EDUCATION

NANOTOUGH – polymers with muscle and a green conscience

Modelling for product-process design within CAPEC

New opportunities for biocatalytic process design and development

Enzyme technology as a research discipline – precision, intensification and bioprocessing

Reducing CO_2 emission in a generic and global perspective

Helping Danish society to use biomass for power production

NANOTOUGH – POLYMERS WITH MUSCLE AND A GREEN CONSCIENCE

Associate Professor Katja Jankova has recently been occupied with the development of polymer materials that hopefully one day soon will replace steel in bumpers for tomorrow's cars. Katja works at the Danish Polymer Centre (DPC) – part of DTU Chemical Engineering. Katja and DPC are involved in a European project, NANOTOUGH, that focuses on developing tough plastic materials using nanotechnology. The perspective is broad and the range of possible applications many – with the automobile and aircraft industries as obvious areas of application. As for bumpers, the benefit is clear – nanocomposite bumpers are as strong as steel bumpers but only weigh about half as much. With a weight saving of 50 kg in medium car, fuel consumption could be cut by approximately 5%.

Like mixing oil and vinegar

Briefly, the developed nanocomposite material consists of two main components – polypropylene (PP) and nanoclay. Both components are inexpensive, but they don't agree with each other; they won't mix. "The problem resembles the well-known household problem with mixing oil and vinegar for a dressing. The oil and vinegar won't mix", explains Katja. "The solution in the nanocomposite is similar to the culinary solution – add a third component to improve the emulsion. For vinaigrette you can use mustard. For a nanocomposite, you have to come up with something a lot more complex – in my case, a block copolymer acting as a compatibilizer." Katja continues: "A block copolymer is a macromolecule, made of two or more blocks of different monomers. The designed new compatibilizer is a diblock copolymer, because it contains two chemically different blocks. For various other applications we have also synthesized diverse triblocks, tetrablocks, and the synthesis of multiblocks is feasible too. The polymers forming the block copolymer structure are as free polymers not compatible with each other - like the polymer (PP) and nanofiller in question used in NANOTOUGH. Especially for the EU project, we have designed, characterized and developed a charged, amphiphilic diblock copolymer, consisting of two blocks, the one having groups anchoring to the nanoclay, the other – miscible/compatible with the PP. This has allowed us to anchor the clay to PP and to better disperse it. Moreover, the mastered diblock material was dispersible in water, and we were able to modify the nanoclay directly in its supplied form – as a 3.6 % aqueous dispersion. After drying, the modified nanoclay was mixed in PP to produce the PP-clay nanocomposite."

Creating the perfect match

"I usually have order in my things. When someone comes and destroys it, this makes me unhappy. After quite a lot of time struggling with the problem, we found that the polymer we used had a similar problem: The PP had strongly confronted with the inserted nanofiller which had broken down its ordered and semicrystalline morphology. Thus, the mechanical properties of the PP had deteriorated. Adding some additives and other fillers (long or short glass fibers) has helped to overcome the problem, and create a novel reinforced NANOTOUGH material.

Katja Jankova wants order in her things and came up with a solution to the problem the nanofiller caused to her polypropylene – thus enabling the development of a reinforced NANOTOUGH material.

Properties similar or superior to steel

PP is a material preferred by the automotive industry for replacement of metal by plastics for reduction of weight and fuel consumption. As concerns weight reduction of load-bearing components, the material properties of the polymer are insufficient. Adding clay together with other additives to the PP nanocomposite has not only improved the bearing load of the components produced so far (bumpers, spare wheel well, dash board), but also stiffness and strength. The time of failure of the PP nanocomposite under creep and fatigue conditions exceeds that of neat PP by at least one order of magnitude. Improvement in barrier properties has also been obtained. The well dispersed nanoclay was found to immobilise significantly the mobility of the polymer

Katja Jankova

Katja Jankova finished her MSc and PhD education at Assen Zlatarov University in Burgas, Bulgaria. Associated Professor in Synthesis of Polymers from the same University. Post doc at the Technical University, Vienna, Austria. From 2000 and presently she is Associate Professor in Functional Block Copolymers at the Danish Polymer Centre, DTU Chemical Engineering. Her research interests are synthesis, functionalization and hydrogenation of polymers and resins – and not least Atom Transfer Radical Polymerization (ATRP). 37 of Katja's 65 scientific publications are fuelled by ATRP. Member of the Editorial Advisory Board of European Polymer Journal (Elsevier).

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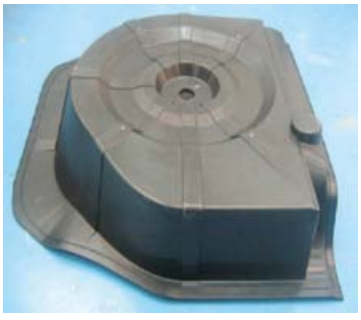


(2)

chains – and hence is also likely to have a positive influence regarding diffusion through a polymer.

Crash test is the acid test

Through an effective collaboration between the partners in the NANOTOUGH project, novel materials have been created. One of the most challenging has been replacing the beam placed behind the automotive bumper. This beam is currently produced by a complex metal construction, welded from different metal parts, with a corresponding high production cost. The prototype for a bumper (1) shows excellent properties with equivalent impact resistance as the metal construction, but with a reduced weight (45%). The bumper beam was successfully evaluated in a crash test at the end of 2011.

A spare wheel well (2), previously produced from a polymer, has now been redesigned and tested – a 50% improvement of the impact strengths was reached, and the well also passed the crash test successfully.

NANOTOUGH project

NANOTOUGH ("Nanostructured Toughened Hybrid Nanocomposites for High performance Applications") is a European framework project that focuses on developing tough plastic materials using nanotechnology. A total of 11 partners from Germany, France, Italy, Spain, Romania and Denmark are participating in the project. Prof. Jesper de Claville Christiansen from Aalborg University is the coordinator of the project. Both DTU and the Danish Technological Institute have been his Danish partners. Among the other partners are Fiat, Ferrari's research centre, and the aircraft and aerospace company Aviospace in Italy. Also participating is Spain's FPK S.A., a part of Mondragon Corporation, who is a subcontractor for VW, Ford, BMW, Audi, Mercedes and Porsche.

Martina Heitzig with fellow PhD student Deenesh Babi and her supervisor Professor Rafiqul Gani, Head of CAPEC centre at DTU Chemical Engineering.

MODELLING FOR PRODUCT-PROCESS DESIGN WITHIN CAPEC

Process systems engineering promotes the solution of problems in a systematic manner. In a changing world, the topics covered within chemical engineering are also changing, influencing thereby, the scope and significance of process systems engineering and its application. In the area of product-process design, the problems differ in terms of the type of chemical(s) being produced. The products and the processes that make them, from petrochemical and chemical industries are usually commodity chemicals, which could be classified as small and/or structurally simple molecules, produced in large amounts. In this case, process optimization in terms of operational efficiency and cost is usually a defining factor for a candidate product-process. The products, and the processes that make them, from life sciences, pharmaceutical, food and related industries, on the other hand, are usually large and/or complex molecules, produced in small amounts. Here, process optimization in terms of operational reliability and time of operation is usually a defining factor for a candidate product-process. This means that although the steps in the systematic solution of product-process design problems could be the same, the models and data, and the methods and tools that employ them in the various solution steps may be very different. Models play a very important role in the systematic solution of product-process design problems. These problems are solved through an appropriate set of methods/algorithms when enough knowledge and/or data are available, which in most cases may not be available. In such cases, models are needed to supplement the available information. For example, models are needed to predict the behaviour of the product-process, to evaluate the performance of the product-process, to monitor and/or control the product-process, and many more. These models may be of different type (different types of equations are used to represent the system); scales (may involve sub-systems requiring different size and time scales); complexity (number of equations, degree of non-linearity, dimension, etc.) and simulation mode (steady state, dynamic, batch, identification, etc.). Issues such as differences in scales of size and time; sources of data and/or knowledge from different disciplines; and, the need to integrate different models, methods and tools to find the optimal solutions need to be addressed. A systems approach that can efficiently "manage the complexity" through a model-data based computer-aided framework becomes therefore a very desirable option.
The PhD-thesis of Martina Heitzig contributes to the development of a model-data based computer-aided framework. The project concentrates on developing a systematic modelling methodology and implements it on a computer-aided framework.

MODELLING THE UNKNOWN

Martina Heitzig works with computer-aided modelling to improve the product-process development cycle. Martina works at the Computer Aided Process Engineering Center (CAPEC) at DTU Chemical Engineering and is currently finishing her PhD. The aim of her PhD project is the development of a computer-aided modelling framework which is based on a systematic modelling methodology in order to make modelling more efficient. In this connection, efficiency means faster model development and more reliable models. The framework is implemented into a user-friendly software by extending the modelling tool 'Modelling Testbed' (MoT) developed at CAPEC.
To achieve more efficient model development, MoT provides computer-aided workflows for different modelling tasks (model documentation, single-scale and multi-scale model construction, model identification/discrimination and model application for simulation and optimization). The workflows provide systematic guidance, are partly automated and integrate the tools and databases needed for each step in the workflows. For example, model construction can be performed in MoT without having to write any programming code, by adding the equations in a simple syntax similar to how equations are written in scientific papers. MoT translates and analyses the equations in order to derive a solution strategy and automatically connects the required numerical solvers. The workflows serve as guidance to the researcher and function as a check list to ensure correct and more reliable modelling.
The modelling framework and the workflows have been developed and refined based on case studies from very different areas within chemical and biochemical engineering.
The MoT software automatically creates reports of all the used workflow steps and their results. This feature is both an advantage to the researcher performing a piece of research and to other potential users of the model.

Predicting how things might work
Martina's modelling work can be illustrated by two examples from real life. An example is pharmacokinetics simulations where the distribution of a drug in an animal or a human is predicted using the models developed through the MoT tool. In this example, data obtained from rats is used to identify the values of the unknown model parameters, and the resulting rat model is scaled up to a human being. In this way, the drug distribution and concentration in the different organs are predicted which can be used for optimising the drug dosage, i.e. administering the drug to the patient in the optimal quantities and intervals. The objective is better and correct treatment of patients.
Another quite different example is the development of fragrance sprays for air freshening. The developed model is able to predict the distribution of the droplets in a room, the size of the droplets due to effects like evaporation, sedimentation (droplets settling due to gravity), convection (the influence of air flow on the droplets' navigation) and agglomeration (merging of droplets) and breaking of droplets.

How Martina ended up at CAPEC and DTU in Denmark
When asked how she ended up at DTU in Denmark, Martina replies "I applied because of ICAS. I found it very interesting that a group (CAPEC, ed.) were developing their own software. I also went because of Denmark, I mean going to a different country and getting to know this country. I heard about CAPEC from a friend in Germany, who was an ERASMUS student with CAPEC then, and later became a PhD student here like me." Martina is finishing her PhD after three years at DTU – her PhD was funded by a DTU scholarship.
Martina believes that "living in Denmark has not been that different from Germany. Naturally, I have had some problems with the language – not reading it, but more speaking Danish", she says with a smile. "I have in particular liked doing my research here, because it's very international at CAPEC." By international, Martina thinks of her colleagues who all have very different backgrounds –be it PhD students, post docs or professors.
When Martina finishes her PhD she will start work at Evonik in Marl, Germany. Evonik is a multinational specialty chemical manufacturer. Martina will work in a department called, CAPE (Computer-aided Process Engineering).

NEW OPPORTUNITIES FOR BIOCATALYTIC PROCESS DESIGN AND DEVELOPMENT

The Center for Process Engineering and Technology (PROCESS) at DTU Chemical Engineering is focused on the development of new and innovative processes for industry. To this end optimization of process design and development plays a key role in saving time and money. An optimized design and development cycle can lead to quicker identification of the processes, reactors, reagents and catalysts that work, and quickly rule out those that will not. Analysis of selected candidates can then be accelerated. For example for biocatalytic processes, the Center has developed an approach that comprises both the process and biocatalyst development sides, thus applying process engineering to biotechnology and chemistry and at the same time integrating these. Likewise, the framework offers a controlled design and development cycle, based on experience and experimental data, which enhances the process and guides further development.

Biocatalysis, the use of cells, enzymes (or parts thereof), is increasingly being used in industry for the synthesis of chemicals. The technology is primarily used in the pharmaceutical and fine chemicals industries but also to an increasing extent for lower value chemicals where high reaction selectivity can be exploited to yield a more competitive process. The main limitations are the limited operating space (e.g. temperature < 100°C) and potentially low productivity (kg product / kg catalyst). When developing a biocatalytic reaction or process, it is therefore necessary to have an understanding of the factors that determine the activity, stability and selectivity of the biocatalyst. Modern biotechnology, on the other hand, offers huge possibilities to improve the biocatalyst, e.g. by directed evolution, to increase temperature stability as well as the activity. However, this is a time consuming activity (and therefore expensive) which is why it is important to have very clear targets for the development of the catalyst and which conditions will be required for an effective and competitive process. At PROCESS, we are developing an approach which uses a range of Process Systems Engineering (PSE) tools (partly in collaboration with CAPEC) to facilitate the development of a biocatalytic process and for guiding the catalyst development.
A simplified development procedure is shown in Figure 1 (p. 26) indicating the interactions between the process and catalyst development efforts and the PSE tools that could be used.

Economic assessment
All business decisions are driven by long or short term economic profitability. Therefore economic assessments at all stages of development should be a part of process selection and design. Although full cost assessments at early stages are not possible due to lack of reliable information about the final process, it is possible to identify critical process parameters and set development targets for the process and biocatalyst based on previous experience or literature data

Professor and leader of the PROCESS Centre at DTU Chemical Engineering, John Woodley (left) and Postdoc, Pär Tufvesson.

for similar processes.
We have previously shown how an assessment of this type could be used to set general biocatalyst productivity targets for different types of biocatalytic reactions, ranging from small scale high value processes for pharmaceuticals to high volume low value bulk process (Tufvesson et al 2011).

Property prediction
The decisions to be made in the implementation of a new biocatalytic process require information on the characteristics of the reaction, the biocatalyst and the equipment/unit operations. Together these three elements constitute the process to be developed. In particular the reaction has characteristics such as the solubility of the compounds involved, the reaction equilibrium, etc. Such characteristics are independent of the biocatalyst but constitute essential information for choice of biocatalysts and operating methods. These data are traditionally obtained from experiments, which are often time consuming. The idea of property prediction is to assist in narrowing down the search space for experimentation.
Together with CAPEC, we have identified that predictive tools for water-solubility and thermodynamics are amongst the most important for the implementation of the next generation of biocatalytic processes. The conditions under which biocatalysis operates make such predictions particularly challenging and provide some interesting targets for future collaborative research.

Operating windows
An operating window is a tool to illustrate the interaction of multiple critical parameters or constraints on the feasibility of a process. There are a number of constraints related to the performance of the process(es) and biocatalyst that will define the operating window. An example is given in Figure 2 (p. 26), indicating some of the limits for operation based on product and co-product concentration, in this case for a transaminase catalysed reaction. Windows

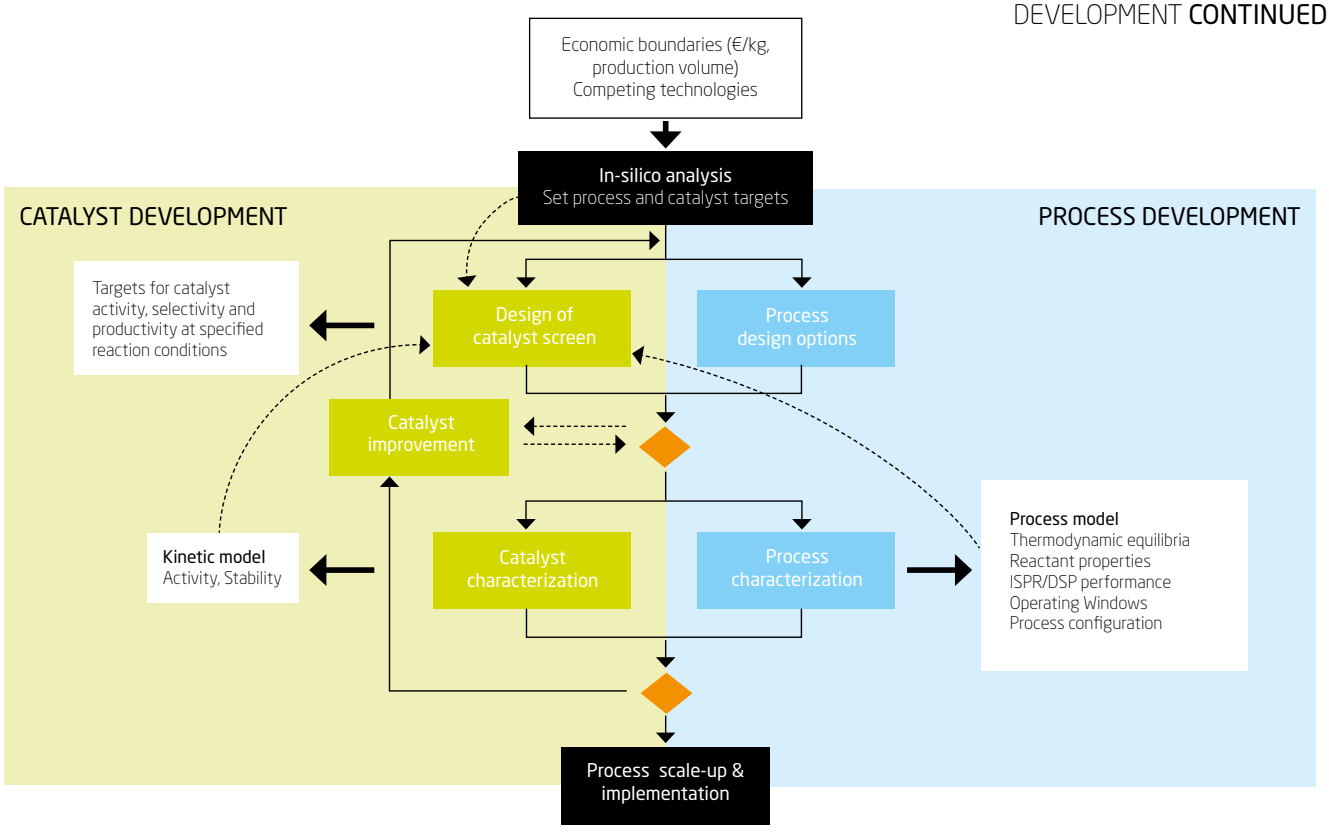


Figure 1

such as this can be used to dictate the requirements on the biocatalyst in the individual case, and also to supply a first guess for the process costs, information that will be very valuable in early development

Micro reactors

PROCESS will deliver a platform miniaturized toolbox that will facilitate the evaluation of different process strategies, using minimal amounts of reactants, catalyst and time. PROCESS aims to demonstrate the feasibility of the micro-scale tools, integrating sensors and new catalysts developed. The results serve as input for building models that can be applied in feasibility assessment and scale up.

Future

The future will see the integration of such tools which will enable rapid and effective implementation of new processes. Collaborative efforts will be essential to develop and integrate the tools. The testing of new methodologies will also be an important activity together with those that implement changes to the biocatalyst (in biological engineering groups) and those that implement retrofit and new dedicated processes (in industry).

TUFVESSON P, LIMA-RAMOS J, NORDBLAD M and WOODLEY JM. 2011. Guidelines and cost analysis for catalyst production in biocatalytic processes. Org. Proc. Res. Dev. 15, 266-274.

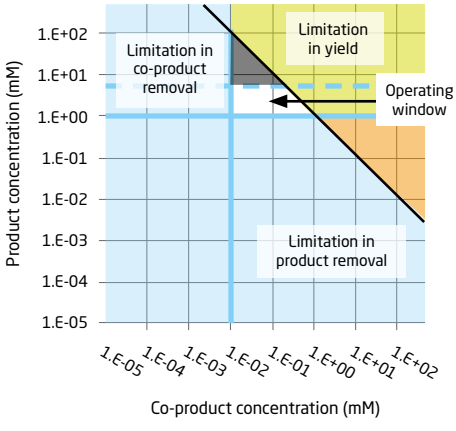


Figure 2

ENZYME TECHNOLOGY AS A RESEARCH DISCIPLINE – PRECISION, INTENSIFICATION AND BIOPROCESSING

Professor Anne S. Meyer, Center for BioProcess Engineering, DTU Chemical Engineering, Technical University of Denmark

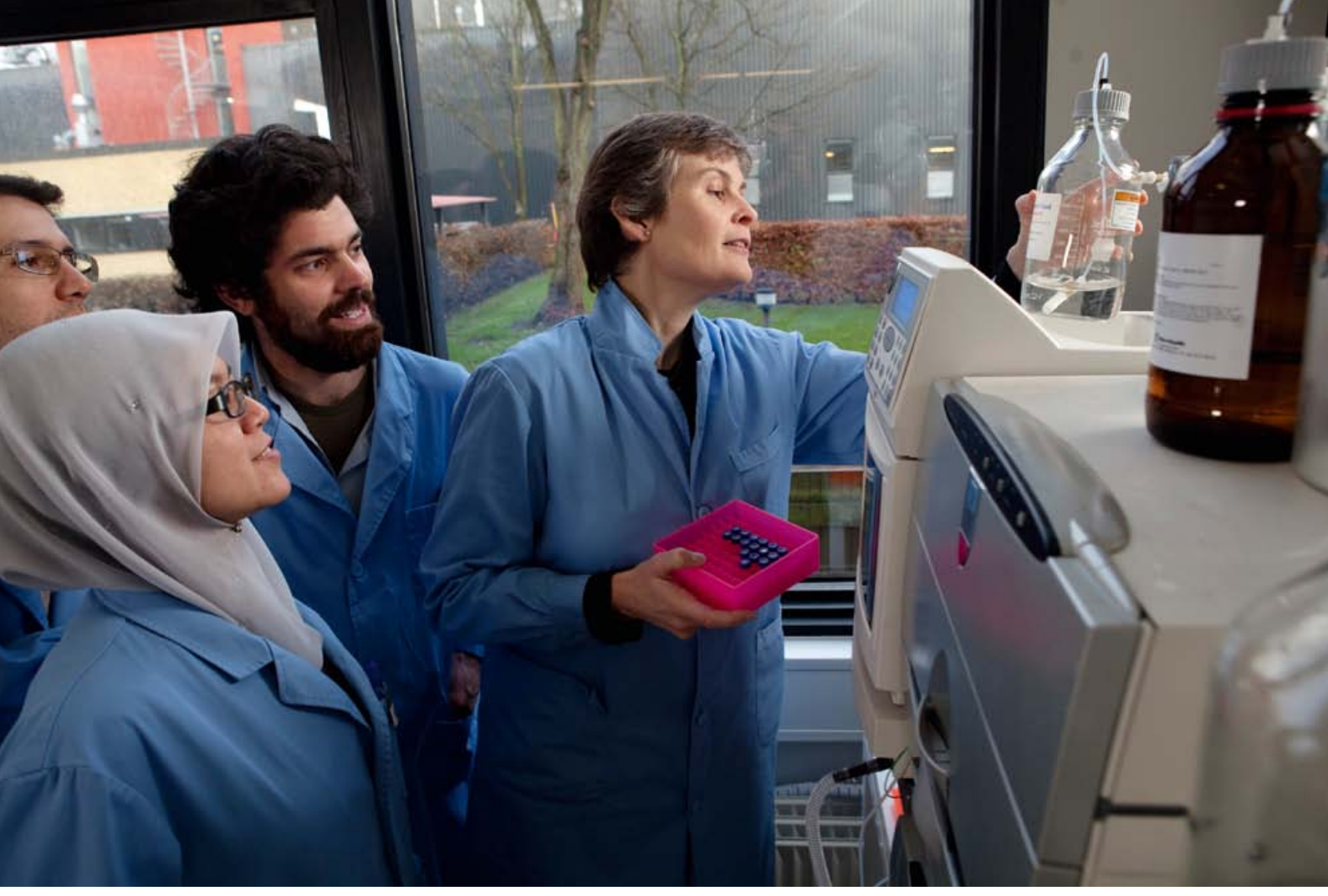
Throughout the world there is a huge demand for precise, intense processes to deliver energy, food, chemicals, materials, and even pharmaceuticals in a sustainable, climate-friendly way. A core requirement is to develop sustainable processes "that meet the needs of the present without compromising the ability of future generations to meet their own needs"1. A key prerequisite for creating such processes is the identification of conversion technologies that are based on green and lean reaction routes that do not require high energy input or involve substances or solvents that compromise human health or pollute the environment. The most immediate need for society is notably to replace fossil oil as a core feedstock, but it is at the same time crucially decisive to enable the production of enough materials, energy, and not least enough food for the world's increasing population. Several new reaction concepts must therefore rely on upgrading of renewable feedstocks.

Enzymes – renewable and biodegradable catalysts

Enzymes are biological proteins that can catalyze different chemical reactions. Enzymes exhibit exquisite specificity and selectivity with respect to the substrates they act upon, the catalytic mechanism, and the reaction route. Like other proteins, enzymes are built of amino acid chains, and the specific sequence of the amino acids making up the protein chain determines the protein's 3D structure, that in turn defines the enzyme's robustness, reaction optimum, and the architecture of the enzyme's catalytic site.

Compared to other catalysts enzymes have a number of remarkable properties that are fit to meet the needs for developing precise and intense conversion processes on renewable feedstocks:

- Catalytic activity under mild conditions
- Specificity / selectivity
- Catalytic activity and stability can be engineered
- Enzymes are renewable and biodegradable
- Most enzymes work best in aqueous systems



Professor Anne Meyer, Center leader at BioProcess Engineering, in the lab with some of her PhD students. Anne Meyer was appointed DTU PhD supervisor of year in 2011.

Since enzymes are catalysts, they provide for a decreased energy of activation for a chemical reaction. The addition of a specific enzyme to a reaction mixture can thus accelerate a slow rate of reaction. In modern enzyme technology, enzymes are mainly used to make certain reactions possible, i.e. to catalyze reactions that are so slow that they do not occur without the enzyme catalysis – one example is enzymatic degradation of cellulose to its glucose constituents. Translated into chemical and biochemical engineering, this means that enzymes can be used to design new conversion processes or help improve the speed and selectivity of existing processes. This is why enzyme technology, encompassing the application of enzymatic catalysis for designing new reactions, processes and products, is a research discipline at DTU Chemical Engineering. The goal of the enzyme technology research at the department is to design innovative products and processes that are competitive as well as sustainable.

Providing research results and skilled MSc and PhD candidates

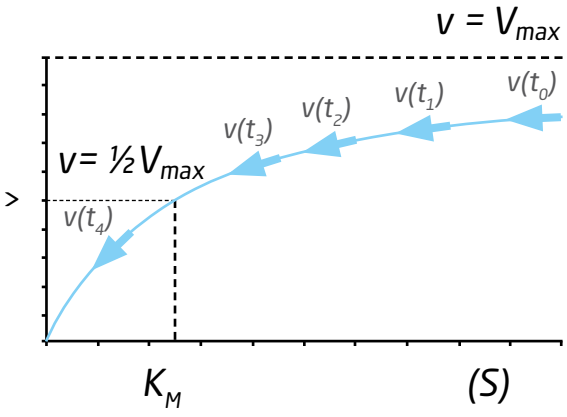
In addition to evaluating new processes, the research discipline of enzyme technology also involves provision of basic knowledge about enzymatic reactions, enzyme structure-function relationships, discovery, design, and production of improved enzymes, unraveling of the enzyme kinetics of different reactions, and extends into definition of new reaction schemes, and use of alternative substrates, processing routes, or reaction schemes, bioreactor design, process technology, and – more recently – sustainability assessment of new processes involving enzyme catalysis.

The more knowledge we can obtain within enzyme technology, the better are our chances for designing new processes and products. The mission is to provide research results – as well as educating candidates with this type of bioprocessing knowledge – for the benefit of both the industry and the society.

[1] Brundtland Commission of the United Nations, March 20 1987; Original definition of sustainability.

ENZYME TECHNOLOGY INNOVATION POTENTIAL

The discovery and development of new enzymes, reactions and products based on enzyme-catalyzed conversions are important applied research objectives that have enormous innovation potential for business development. Completely new processes such as conversion of lignocellulosic biomass components into value-added products, targeted extraction of prebiotics from agro-industrial by-product streams and enzyme-assisted synthesis of bio-functional food ingredients are examples of a novel type of sophisticated, enzyme-catalyzed reactions that can help build better and more sustainable products. Enzyme-based solutions can clearly address some of the most critical global challenges and enzyme technology is therefore a key enabling technology for the future.



Graphics acknowledgment: Michael Krogsgaard Nielsen

In the past year, project work in the Center for BioProcess Engineering at DTU Chemical Engineering has:

1.
Established a new concept involving targeted enzyme based polishing of low value pectin to obtain defined molecular products (having distinct bioactivity)

2.
Discovered how the thermal stability of certain enzymes depend on the hydrogen bonding capacity of the solvent anion in ionic liquids

3.
Developed a new lean enzymatic process for selective release of biofunctional fibers from an agro-industrial byproduct stream

4.
Identified the specific amino acids in the sequence of pectin lyase being responsible for the enzyme's pH optimum

5.
Discovered a new heat tolerant pectin degrading enzyme

6.
Identified a NIR based methodology to predict enzymatic hydrolysis of differently pre-treated biomass

7.
Conceived several new conversion routes for production of new products - currently being further explored.

REDUCING CO_2 EMISSION IN A GENERIC AND GLOBAL PERSPECTIVE

The emission of CO_2 is a global problem. It is produced in large part from agriculture, transport and the industry. At Applied Thermodynamics Center for Energy Resources Engineering (AT CERE), DTU Chemical Engineering, software tools, methods, experiments, and pilot facilities are developed in the battle for reducing the impact of global warming and supporting an industrial focus. DONG Energy and Vattenfall A/S have recently participated in close collaboration in several projects on simulation and optimisation of the CO_2 capture processes. AT CERE at DTU Chemical Engineering is continuing the development of advanced technologies in several large EU funded projects.

CO_2 capture is a technology which can help reducing emissions of CO_2 from the power, iron, cement, and bio industries. Denmark can reduce its emission by 40% by applying the technology, the equivalent of 21 million ton of CO_2 per year.
Currently, Denmark is embracing the possibilities of renewable energy in terms of wind power. Scandinavia is becoming a leader in the game of renewable energy, while the remaining world is still bound to use coal. It is available in large amounts in USA, China, Russia and Australia. Coal resources can last for at least 100 years, and the cost of energy is low compared to renewable energy. The risk is high, and thus the need for knowhow, which is not present in all parts of the world.

Philip Loldrup Fosbøl has been involved in several of the CO_2 projects and has recently been appointed Assistant Professor at DTU Chemical Engineering. "In Australia, they are literally extracting the coal off the side of a mountain, using shovels. Can a renewable technology compete with that? Most likely, the coal will be burnt, especially by countries which are not able to construct and maintain renewable technology." explains Fosbøl. "Denmark needs to be active not only in renewable technology, but also in seeing the market potential for developing CO_2 capture technologies for the future".

Method applied in industry
Since 2003, a tool has been developed for post-combustion capture. Jostein Gabrielsen initialised the work during his PhD on a software package, which was later expanded and generalised by Philip L. Fosbøl and used by Leila Faramarzi in her PhD. Through close collaboration with DONG Energy and Vattenfall, a common interface was formulated allowing the industry to use the software in a more generic sense. Now, Vattenfall has proved the concept of estimating and optimising a complete power plant fitted with CO_2 capture technology in their in-house software, which allows for energy and cost reduction. The Danish Strategic Research Council is supporting the initialisation of basic communication between the research partners, which is beneficial for the end product.

"Accuracy of the developed software is of utmost importance", Philip Fosbøl states.
This is obtained by using an advanced mathematical model developed by Associate Professor Kaj Thomsen. "The model is a general thermodynamic tool for electrolytes. It can be used in a number of calculations of electrolytes applied to e.g. scale prediction, flue gas desulfurization, acid gas treatment, wastewater treatment, or compatibility of product formulation. We have a unique tool, which can be used by all users to calculate salt solutions. We even have a plug-in for process simulators like Aspen Plus", says Kaj Thomsen as he explains how Negar Sadegh is using the model in her PhD studies of acid gas treatment.

Since 2008, Kaj Thomsen has supervised several PhDs on CO_2 capture in innovating the solvents used in CO_2 capture. Victor Darde is one of the recently graduated students who has finalised a very

From left: Philip L. Fosbøl, Kaj Thomsen, and Nicolas von Solms discussing the CO_2 capture pilot at DTU Chemical Engineering, developed by skilful students.

detailed study on the chilled ammonia process (CAP), using precipitating ammonia. Nutritious amino acids are also being studied by Benedicte Mai Lerche for the purpose of promoting CO_2 capture. "Your health could actually improve if you ate the solvent", Lerche adds. Another solvent being studied for carbon capture and storage (CCS) purposes is ionic liquids which are often used in catalysis. In collaboration with DTU Chemistry, Subham Paul has proven that there is a potential in applying ionic liquids for CO_2 capture using a standardized method, which could revolutionise the CO_2 capture business. At DTU Chemical Engineering, Sharat Kumar Pathi is studying the field of high-temperature CO_2 capture by carbonate looping relevant for the cement industry.

Today, research is carried out in several FP7 EU projects. The CESAR/CLEO DTU project focuses mainly on simulation. "We are able to accurately predict the results of the CASTOR EU project without data correlation, using our $CAPCO_2$ software", Philip Fosbøl notes. Associate Professor Nicolas von Solms is maintaining the project leader role of the EU iCap project (Innovative CO_2 Capture). Von Solms supervises Peter J. Herslund in one of many research projects on gas hydrates. The intent is to actively promote the formation of CO_2 hydrates in the capture process. Muhammad Waseem Arshad is also participating in the same project studying phase change solvent by liquid split phenomena in order to develop the CO_2 capture technology.
Nicolas von Solms' main focus has been to attract skilled students for construction of a pilot scale CO_2 capture facility. "We have just taken on two new students to finalise the design of the desorber column for the DTU Chemical Engineering capture pilot".

During the coming year, the EU OCTAVIUS project will be initialised. DTU's leading role will be to develop a generic tool for CO_2 capture process simulation based on the CAPE-Open standard.

Transportation
CO_2 from a capture process often needs to be carried from the production facility and downstream. This is typically transported in pipes or by ship. In this connection, securing flow integrity is essential. During 2008, Philip L. Fosbøl finalised his PhD on CO_2 corrosion phenomena and ways to improve corrosion modelling in close collaboration with Maersk Oil. Philip L. Fosbøl explains, "During the coming years, several projects, already financed, will be initialised on the corrosion aspects of CO_2."

Energy from CO_2 storage
CO_2 is often being seen as a waste product. Ben Niu recently finalised his PhD., supervised by Alexander Shapiro, and continued into a postdoctoral position in the center on CO_2 injection into oil reservoirs as one of many projects in this area. The purpose is to increase the oil production and at the same time bring the CO_2 back to its original place in nature.

HELPING DANISH SOCIETY TO USE BIOMASS FOR POWER PRODUCTION

The CHEC (Combustion and Harmful Emission Control) centre at DTU Chemical Engineering has over the last 15 years performed research on biomass combustion, which is viewed as a key element to obtain a CO_2 neutral production of power and heat. Danish central power plants are planning in the near future to reduce the use of coal and mainly apply biomass fuels. Biomass fired power plants can ensure a renewable and load adaptable electricity production, while other renewable electricity producers, such as windmills, are dependent on daily climatic changes.

Biomass boiler combustion issues

Danish power plants now have to reduce the use of coal and mainly apply biomass on the central power plants – this is decided by the Danish government as one of the initiatives to reduce greenhouse gas emissions and reduce the use of coal for power production. In a continuing effort, the CHEC research centre collaborates with the Danish power plant companies to obtain reliable and efficient power production based on biomass combustion. This collaboration was initiated in the mid-90's where CHEC participated in the first full-scale tests of co-combustion of coal and biomass. Nowadays, the aim is to completely replace coal with biomass at the central plants.

Upgrading large pulverized-fuel fired power plant boilers, designed originally to use coal, to utilize biomass is not a trivial task. It is difficult to grind biomass down to particle sizes similar to coal particles so fuel handling and flame properties change when straw or wood fuels are used. Furthermore, the inorganic elements in biomass give rise to an ash that often causes problems with deposit formation in the boiler chamber, corrosion of boiler coils, and reduction of the efficiency of flue gas cleaning equipment.

Ash deposition

As part of an Energy.dk financed project, PhD student Muhammad Bashir has together with his supervisors developed an advanced ash deposit probe technology that can be used to measure and quantify deposit formation and removal in biomass fired boilers. The measurements include an in-situ registration of the amount of deposit and a video registration of the deposit formation process. Probe measurements were conducted on the Vattenfall owned Amagerværket unit 1 boiler, the only suspension fired boiler using straw as fuel without co-firing, and on DONG's Avedøreværket 800 MWth wood fired unit 2 boiler. The probe measurements provided quantitative deposit formation rate data and showed that increased local flue gas temperature and increased fuel K-content cause increased deposit formation rate, while the coil surface metal temperature only influences the initial deposit build-up. The actual build-up of deposits is controlled by formation and shedding processes. Increased coil surface temperature and maturation of deposits cause a higher soot blower jet peak impact pressure to be required in order to remove the deposit. The project results make it easier to predict the influence of local boiler conditions and biomass type on ash deposit behaviour.

Professor Peter Glarborg (left) is head of the GREEN research centre financed by the Danish Council for Strategic Research. Associate Professor Peter Arendt Jensen has managed the power plant deposit probe investigations.

Power Generation from Renewable Energy (GREEN)

In 2011, the GREEN research centre, a collaboration between several universities and the companies DONG Energy, Vattenfall, and Burmeister & Wain Energy was initiated, funded by the Danish Council for Strategic Research. It is managed by Professor Peter Glarborg from the CHEC centre, and the main objective is to facilitate the design of future flexible and efficient thermal power plants using 100% bio-dust firing.

The GREEN centre ambition is to ensure a leading position for both Danish power industry and Danish research groups regarding use of biomass in power production. In the project, CHEC deals with improved burner design for flame stability and fuel flexibility, development of efficient deposition/corrosion control methods, and minimization of flue gas cleaning catalyst deactivation. In addition, DTU Mechanical Engineering looks into development of novel super-heater materials to resist high-temperature corrosion and Aarhus University aim to refine agricultural techniques to yield biomass fuels (in particular dedicated energy crops) better suited for use on central power plant units.

A broad range of research methods will be used. A collaboration with Lund and Stanford universities boosts efforts to develop improved models for biomass particle conversion. The models that describe biomass particle ignition, devolatilisation, and char combustion will be evaluated by use of measuring data obtained on a single particle combustion reactor and on an entrained flow reactor. To investigate biomass flame characteristics advanced optical measurements will be conducted on several full-scale swirl-stabilised biomass burners. A main objective is to investigate the influence of burner operation conditions on flame stability. The obtained data will be analysed by comparison with CFD calculations of the flames. A detailed study on the fly ash formation process will also be conducted. The fly ash strongly influences deposit formation and corrosion processes. It is the objective to obtain a comprehensive ash transformation computer model by combining models of the fly ash formation process with a deposit formation model. Verification of the model will be done with both full scale deposit probe measuring data and laboratory entrained flow reactor measurements on ash transformation.

ORGANIZATION

DPC

CHEC

CAPEC

BIOENG

PROCESS

AT CERE

Service Center

Photo taken at our Annual Christmas Meeting at which we welcomed our new colleagues from Risø.

At the Danish Polymer Center we are devoted to the application of molecular design, synthesis and processing of polymers to create materials and products with unlimited ranges of properties and applications. We strive towards this goal in a balanced environment of education, research and industrial cooperation.

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DPC

THE DANISH POLYMER CENTER

The Danish Polymer Center (DPC) is devoted to fundamental research in polymers, soft materials and complex fluids. The aim is to utilize polymer research in education, technological innovation and industrial collaboration. Organized within DTU Chemical Engineering, the center is located in newly refurbished laboratories in Building 227. The research is interdisciplinary, ranging from chemical synthesis, chemical and physical characterization of polymers and soft materials, to fluid mechanics of complex fluids.

Equipped with state of the art instrumentation for polymer characterization, the laboratories at DPC provide a common ground for polymer chemists, polymer physicists and chemical engineers. Current techniques include the synthesis of polymers with controlled molar mass, branching structure and functional groups, application of scattering methods for study of complex polymer systems, rheological characterization and the design of multi-phase systems.

MSc in Polymer Engineering
Students in the DTU Master's Program in Advanced and Applied Chemistry may specialize in Polymer Engineering. This will allow master students to be trained in our laboratories and to engage in research at DPC.

Research Consortium in Polymers at DTU
The basic purpose of this consortium, established in 2006, is to ensure both stability and continuity of contact and communication between DPC and the parts of Danish industry that commercially use polymers. The consortium will run a number of smaller research projects and will serve as a greenhouse for conceiving ideas and innovating plans for future research and educational initiatives.

Graduate School Program in Polymer Science
Initiated in 2003, the Graduate School of Polymer Science is a research education network between the DTU Chemical Engineering, the Department of Chemistry at Aarhus University, Risø National Laboratory and other associated industrial companies.

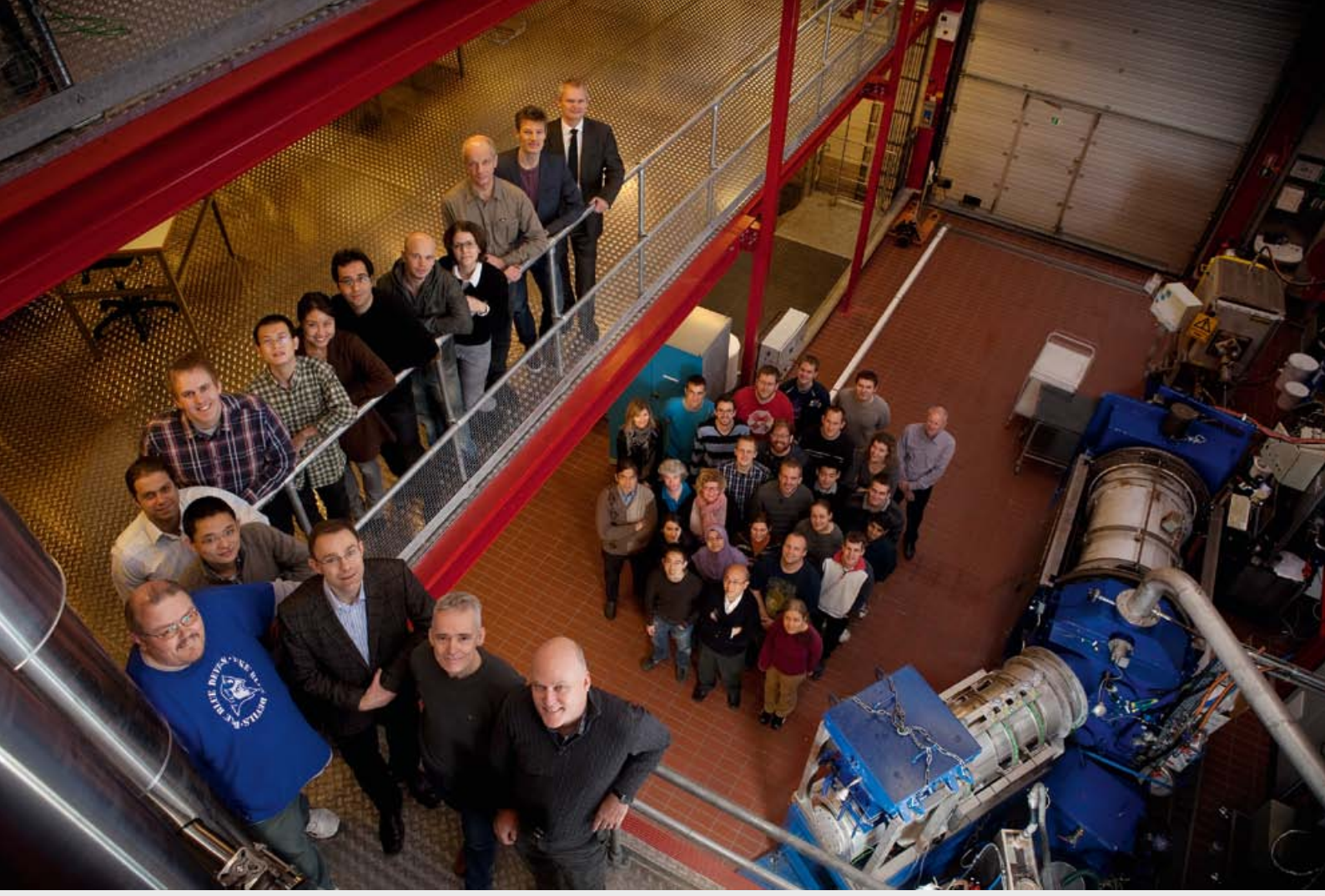
Financial support
Financial support to the DPC is provided by the Danish National Research Council, the European Union, the members of the Research Consortium in Polymers and the members of the Graduate School in Polymer Science.

Members of the Graduate School Program of Polymer Science are as follows

- Coloplast A/S
- Elektro-Isola A/S
- Grundfos A/S
- Novo Nordisk A/S
- Radiometer Medical ApS
- Teijin Twaron

Members of the Research Consortium in Polymers are as follows

- Alfa Laval Nakskov A/S
- Coloplast A/S
- Dana Lim A/S
- Dyrup A/S
- Grundfos Management A/S
- Hempel A/S
- Novo Nordisk A/S
- Radiometer Medical ApS
- Tetra Pak Packaging Solutions AB



A vital part of our research is conducted in very close collaboration with industrial enterprises and international research organizations. The industrial relations cover close joint projects with a mutual exchange of staff and cooperation on experimental research ranging from microscale over pilot plants to full-scale industrial production plants. This approach ensures high relevance of our research and efficient exchange of technology, know-how and know-why.

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CHEC

COMBUSTION AND HARMFUL EMISSION CONTROL – THE CHEC RESEARCH CENTER

CHEC is a research center mainly focused in the field of Chemical Reaction Engineering and Combustion, emphasizing high-temperature processes, formation and control of harmful emissions, catalysis, particle technology and product design.

The research approach involves a combination of modelling and experimental work. Experiments are conducted over scales ranging from small laboratory reactors to full-scale industrial units.

Mathematical models typically combine a generic description of the chemical reaction system with a process-specific flow. They are used to analyze and extrapolate the experimental data as well as providing input for design and optimization.

The work is conducted in collaboration with enterprises and a range of national and international research organizations.

The research in product design covers quantitative formulation engineering using traditional chemical engineering methods in the design of products such as granular enzymatic products, and controlled release systems, in many different fields. Special emphasis is put on advanced heavy duty coatings.

Combustion of alternative fuels for heat and power production remains an important research field in CHEC, with current emphasis on facilitating use of biomass in the central power plants and new fuels in the cement industry. Furthermore, waste fuel utilization, methods to reduce CO_2 emissions, and production of liquid fuels from biomass have received increasing attention in the CHEC Research Center over the last years. The work conducted is also directed towards pyrolysis of biomass, oxyfuel combustion and gasification.

Within catalysis, the work focuses on synthesis of fuels such as methanol and higher alcohols from syngas, upgrading and steam reforming of biomass pyrolysis oils and catalytic reduction of emissions from power stations and vehicles. Recently, fuel cell/electrolysis technology has also been studied.

Together with the pharmaceutical industry the CHEC capabilities within chemical reaction engineering and advanced experimental techniques are used to establish new continuous production processes.

The CHEC Research Center collaborates mostly with the following industrial partners

- Babcock & Wilcox Vølund ApS
- B&W Energy A/S
- Danish Gas Technology Center A/S
- DONG Energy A/S
- Energinet.dk
- FLSmidth A/S
- H. Lundbeck A/S
- Haldor Topsøe A/S
- Hempel A/S
- Hwam A/S
- MAN Diesel A/S
- Novozymes A/S
- Topsøe Fuel Cell A/S
- Vattenfall AB

Briefly, the research objective of CAPEC is to develop computer aided systems for process simulation, process/product synthesis, design, analysis, and control/operation that is principally suitable for the chemical, petrochemical/oil, pharmaceutical, food and biochemical industries.
Our computer-aided systems are developed on the basis of fundamental modelling studies that incorporate estimation of thermophysical and phase equilibrium properties as well as description of the underlying phenomena and behavior of the processes and operations. We manage the complexity related to the solution of a wide range of product-process development problems in product and process engineering and contribute to innovative and sustainable technologies.

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CAPEC

COMPUTER AIDED PROCESS-PRODUCT ENGINEERING CENTER (CAPEC)

The CAPEC research center applies a systems engineering approach to develop comprehensive solutions to various industrial problems based on a thorough analysis of scientific issues and actual product/process requirements. The developed systematic methods are generic in character and therefore applicable to a wide range of problems in traditional chemical and petrochemical industries as well as to solving problems in emerging areas including life sciences (nutrients, health, medical sciences, biotechnology, and bio fuels), pharmaceutical industry, food industry, energy, and enterprise-wide optimisation.

Additionally, the systems approach enables CAPEC to convert the developed methods into software tools for problem analysis and solution. Thus, the research at CAPEC has resulted in the development of a range of generic model based techniques and their conversion into state of the art computer-aided tools for modelling, synthesis, design, operation, control, and analysis – each method dedicated to systematic and efficient process-product engineering.

The research at CAPEC is organized into six research programs within a logical framework ranging from fundamental to applied research. Based on the fundamental modelling at the generic levels, computer-aided methods and tools are developed at the next (intermediate) levels for synthesis, design, analysis, and control of process/product/operation. Again, these models, methods and tools are integrated in the final research levels, where end-user solutions are generated for the development of cleaner, safer, innovative and sustainable technologies.

Headed by Professor Rafiqul Gani, the CAPEC research center constitutes a very distinct group of professors and associate professors, researchers, postdocs, and PhD students that contribute to the joint activities of DTU Chemical Engineering. Members of two research groups (Systems Engineering and Process Technology within DTU Chemical Engineering) now contribute to the products and services offered by CAPEC. Additionally, CAPEC usually hosts around ten MSc and BSc students plus a varying number of visiting students and international visitors.

In 2011 CAPEC was supported by the following industrial consortium

- Akzo-Nobel (NL)
- Alfa Laval A/S (DK)
- AstraZeneca (S)
- BASF (D)
- Bayer AG (D)
- Borealis Polymers Oy (SF)
- ChemProcessTechnologies (USA)
- Chemtura Netherlands B.V. (NL)
- Céondo Ltd. (UK)
- ConocoPhilips Company (USA)
- Danisco A/S (DK)
- DSM (CH)
- Firmenich (CH)
- FMC Corporation (USA)
- GlaxoSmithKline (USA)
- Huntsman Europe (NL)
- Invensys SimSci-Esscor (USA)
- Kongsberg Oil and Gas (NO)
- Lonza AG (CH)
- Mitsubishi Chemical Corp. (JPN)
- Navadan (DK)
- Neste Oil (SF)
- Novozymes A/S (DK)
- Optience (USA)
- Petrobras (Brasil)
- Processium (F)
- ProSim (F)
- SCG Chemicals Co. Ltd. (TH)
- Syngenta (UK)
- Unilever (USA)
- VTT Technical Research Centre of Finland (SF)

The goal of the Center for BioProcess Engineering is to create a strong link between generic chemical engineering research and the industrial application of biotechnology.

The vision of the Center is to provide new knowledge led principles for designing new, biobased production processes and products. At the same time, the objective is to hatch top-qualified M.Sc. and Ph.D. candidates through research based teaching and supervision. We hope that this twofold strategy will contribute to fulfilling the potential of biotechnology to substantially impact industrial production and thereby contribute to development of new, ingenious, and sustainable processes and products.

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BIOENG

CENTER FOR BIOPROCESS ENGINEERING

The purpose of the Center for BioProcess Engineering is to strengthen the integration of chemical engineering research with biotechnology via a focused research effort linking generic chemical engineering science with applied biotechnology. The Center operates at the interface between biotechnology and chemical product and process engineering with a particular research focus on processes involving biocatalytic reactions, and thus the research discipline Enzyme Technology. A main vision of the Center is to develop new, specific biorefining routes for improved raw materials utilization and production of new biochemicals, platform compounds, biofuels, and food ingredients by use of biocatalysis and to contribute to establish DTU as an internationally recognized University within the fields of enzyme technology and bioprocess engineering.
The research is structured into four research subjects: **1**) Enzyme Discovery and Cloning; **2**) Enzyme Assays and Kinetics; **3**) Enzyme Reaction Design; **4**) Reactor Design and Separation Technology. Transverse enabling technology platforms include: A) Enzyme production; B) Analytics. The Center for BioProcess Engineering hosts the following large research structures:

Center for Biological Production of Dietary Fibres and Prebiotics was established in 2007 via a grant from The Danish Council for Strategic Research. The research focus is on developing bioconversion processes for upgrading of low-value agroindustrial plant streams to high value carbohydrate products having potential health benefits. The research involves significant and close collaboration with two international companies, Herlev Hospital, and other DTU Departments.

The Human Milk Oligosaccharides Programme was initiated in 2010 as a larger research effort on a grant from The Danish Council for Strategic Research. The research concerns the enzymatic design of bioactive human milk oligosaccharides and takes place in collaboration with industrial and academic partners, notably Arla Foods amba, DuPont Nutrition & Health, University of Reading; Southern Danish University, Copenhagen University and DTU Chemistry.

The Center for BioProcess Engineering also participates in the *Marie-Curie ITN Lean Green Food Programme* involving education of 13 PhD students, 4 of them enrolled at DTU. It is an imperative necessity for the food industry to develop new production systems to meet global challenges related to environmental awareness, sustainability and consumer expectations. The challenges involve designing new processes for better utilization of natural resources to create high-added value products from biomass/agricultural raw materials with less water consumption, reduced energy expenditure and limited use of chemical reagents and synthetic ingredients. In the *Lean Green Food Programme* the focus is on designed enzymatic modifications to meet these challenges.

Center for BioProces Engineering currently collaborates with the following industrial partners

- Arla Foods Amba
- Chr. Hansen A/S
- DuPont Nutrition & Health
- DONG A/S
- Foss Analytical A/S
- Grundfos A/S
- KMC
- Lyckeby Stärkelsen Amba (Sverige)
- Novozymes A/S
- Novo Nordisk A/S

The vision of the Center for Process Engineering and Technology is to provide the necessary support to enable the nextgeneration of processes to be implemented in industry. In this way, the new developments in biotechnology, catalysis and separation science alongside process engineering can be translated into industrial practice. New processes with reduced waste, high efficiency, and based on all the principles of sustainability can be developed which will help develop the European industrial sector in the production of chemicals, bio-based materials and chemicals, as well as pharmaceuticals.

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PROCESS

CENTER FOR PROCESS ENGINEERING AND TECHNOLOGY

The Center for Process Engineering and Technology (PROCESS) is focused on the development of new and innovative processes for industry – so-called 'next-generation processes'. PROCESS works at the interface of a number of disciplines, including biotechnology, process engineering and chemistry. The objective is to provide the necessary infrastructure and support to evaluate and implement the next generation of processes in the chemical, bio-based and pharmaceutical sectors in particular. The research is carried out in close collaboration with industry and work is carried out at three levels, namely: laboratory scale experimental process evaluation; model based evaluation of process technology and pilot-scale process validation. Three demonstration units operate in the pilot facilities, one for immobilized enzyme reactions, one for enzymatic biodiesel production and one for organic synthesis. Using the results from work at the three levels enables new technology and processes to be evaluated both experimentally and also from the perspective of implementation. The Center is involved in the following large collaborative projects in Denmark and in Europe:

Sustainable Biodiesel is a project established in 2008 with the Danish National Advanced Technology Foundation, DTU Management, Novozymes A/S, Aarhus University and Emmelev A/S. It is focused on developing a new enzymatic route to biodiesel. In 2011 a pilot plant to demonstrate the enzymatic production of biodiesel was built in building 228.

Towards Robust Fermentation Processes by Targeting Population Heterogeneity at Microscale is a project established in 2009 with the Danish Council for Strategic Research, DTU Systems Biology, DTU Fotonik, Department of Biology (University of Copenhagen), Department of Biotechnology, Chemistry and Environmental Engineering (Aalborg University), Crystal Fibre A/S, Fermenco ApS and Foss A/S. It is focused on characterization and control of the heterogeneity of a population of microorganisms in a fermentation.

In the *pharmaceutical* sector, several projects sustain the development of the next generation of enzyme based methods for the synthesis of optically pure molecules (including 'AMBIOCAS', 'EngBiocat', 'BIOTRAINS' and 'BIONEXGEN' funded by the EU, and 'Continuous Microfactories' funded by the Danish Council for Independent Research – Technology and Production Sciences). The Center is also involved in a 5-year project with Lundbeck, aiming at moving from batch towards continuous production, and is a partner in the F3 European consortium established in 2009. The main focus of F3's activities is the creation of novel production process technology for the development of early stage pharmaceutical leads in collaboration with AstraZeneca Ltd.

The PROCESS Research Center collaborates primarily with the following industrial partners

- AstraZeneca Ltd (UK)
- BASF SE (D)
- BioSilta Oy (SF)
- Bioingenium SL (ES)
- Britest Ltd (UK)
- CLEA Technologies BV (NL)
- c-Lecta GmbH (D)
- Crystal Fibre A/S (DK)
- Emmelev A/S (DK)
- Evonik Industries AG (D)
- Fermenco ApS (DK)
- Foss A/S (DK)
- Haldor Topsøe A/S (DK)
- Ingenza Ltd (UK)
- Novozymes A/S (DK)
- Royal DSM NV (NL)

In 2011 PROCESS formally became part of the CAPEC-PROCESS Industrial consortium to further strengthen the application of CAPEC tools in PROCESS related projects.

For more than 30 years the Center for Energy Resources Engineering (CERE) has been a leading research group in the area of applied thermodynamics (previously known as IVCSEP). In close collaboration with industry, relevant authorities and international research organizations, the scientific results from CERE are implemented in industrial products and processes.

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AT CERE

APPLIED THERMODYNAMICS - CENTER FOR ENERGY RESOURCES ENGINEERING

AT CERE is the section of CERE at DTU Chemical Engineering.
CERE was created in 2009, as a continuation and extension of the IVC-SEP center, and has activities across DTU. At DTU Chemical Engineering the main contributions are within the area of applied thermodynamics and transport in porous media. In close collaboration with industry, relevant authorities and international research organizations, the scientific results from AT CERE are implemented in various industrial products and processes.

CERE is a strategic effort at DTU which combines expertise in applied thermodynamics, colloids & interfaces, geoscience and scientific computing. CERE has nine faculty members, of which five are at DTU Chemical Engineering.
The main activities of AT CERE are in the areas of complex solutions (including polymers, electrolytes, peptides, and associating chemicals), nonequilibrium thermodynamics (diffusion and thermo diffusion), and simulation of petroleum recovery processes. These skills are applied in several research projects of strategic importance such as CO_2 capture and storage, flow assurance and Enhanced Oil Recovery (EOR).

CERE's Industrial Consortium is a valuable asset for research and education at DTU. Many companies provide financial support for research projects in addition to the membership. For instance the Chemicals in Gas Processing project (CHIGP), which is extensively sponsored by industrial partners (Statoil, Gassco, DONG Energy, BP and Maersk Oil).

In 2011, several CERE projects were initiated with significant contribution from DTU Chemical Engineering. Three major novel research projects were:

- *SmartWater*. The project will study chemically modified water as an easily accessible and sustainable method for EOR. The project is funded for a 4-year period by the EUDP (under the Danish Ministry of Climate and Energy), Maersk Oil and DONG Energy.

- *BioRec - Biotechnology in Oil Recovery* - is a unique partnership between oil and biotechnology, represented by Maersk Oil and DONG Energy - and Novozymes, respectively. This is a 4-year project, funded by The Danish National Advanced Technology Foundation, Maersk Oil and DONG Energy.

- *CO_2 Hydrates – Challenges and possibilities* is a collaboration with Ecole des Mines in France. The project received funding from the Danish Council for Independent Research.

Another rapidly growing activity is the research concerning post-combustion CO_2 capture. Within this area the center are involved in several projects and extensive EU collaborations.

In 2011 the Industrial Consortium consisted of the following members

- Akzo Nobel (NL)
- BP (GB)
- Chevron (US)
- Conocophillips (US)
- DONG Energy A/S (DK)
- Eni (IT)
- ExxonMobil (US)
- GASSCO (NO)
- GDF-SUEZ (FR)
- Haldor Topsøe (DK)
- Linde (DE)
- Maersk Oil (DK)
- Petrobras (BR)
- RWE (DE)
- Saudi Aramco (SA)
- Schlumberger (US)
- Shell (NL)
- Sinopec (CN)
- Statoil (NO)
- Total (FR)
- Vattenfall A/S (DK)
- Welltec (DK)
- Lloyd's Register ODS (DK)
- IFP (FR)
- OMV (AT)

Our support units provide important services for students, teachers and researchers and are responsible for the full array of technical and administrative functions at the department.

It is our mission to provide professional, smooth and flexible support and service to the rest of the department and towards partners both inside and outside the Technical University of Denmark.

Deputy Director,
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SERVICE CENTER – TECHNICAL AND ADMINISTRATIVE SUPPORT

THE SERVICE CENTER AT DTU CHEMICAL ENGINEERING COMPRISES SEVEN SERVICE AND SUPPORT UNITS. THROUGH THE VARIOUS UNITS, THE SERVICE CENTER SEEKS TO SUPPORT THE DEPARTMENT'S EDUCATION AND RESEARCH ACTIVITIES. THE SERVICE CENTER IS MANAGED BY THE DEPARTMENT'S DEPUTY DIRECTOR, KARSTEN HJORTH REICHSTEIN.

SERVICE AND SUPPORT IS DELIVERED BY:

HR

The HR function's primary objective is to support the department on personnel issues and tasks. The function supports the department's management on hiring and recruiting new personnel, introducing new personnel, preparing and defining HR-related guidelines and policies. Other focus areas include international work relations, work environment issues and holidays and absence handling. The local HR function has wide cooperation with the central HR function at DTU.

IT

The IT team provides local support for the employees of the department. Support includes general pc support and user support, creation and management of IT users, software management and updates and audio visual equipment. The local IT team also handles contact and cooperation with DTU central IT administration and external vendor – in which IT infrastructure implementation and operations reside and are managed.

FINANCES

The central finance administration at DTU provide financial staff who work with center leaders and project managers on funding, financial project administration, project support, financial controlling and reporting, financial key figures, budgeting and financial reporting. The primary focus is to ensure safe and smooth financial management at the department.

PROJECT SECRETARIAT

The Project Secretariat supports the management of the department on areas including internal and external communication, cross-departmental projects, management information and reporting. Practical tasks include support for strategy work and plans, annual reporting for DTU central administration – and on communication, the preparation of the Annual Report, management and update of website, internal newsletter and intranet.

CUSTOMER SERVICE

Customer Service comprises reception and janitor services. The unit handles physical mail, meetings, guests and visitors, photocopying, phones and a wealth of practical issues to support the working day of the rest of the department.

STUDENT ADMINISTRATION

The primary focus area is general student administration, including support for students, researchers and faculty. The unit also provides secretary support for various committees on research, innovation and teaching, including Summer University and Departmental Seminars.

WORKSHOP AND PILOT PLANT FACILITIES

The workshop features modern and well-functioning facilities. The workshop plays a basic and supportive role in the department's core activities on education, research and development within process and production technology and chemical product development – servicing both private and public institutions and organizations, domestic and international.

LABORATORIES

Our laboratory technicians ensure high safety standards and efficient caretaking of our laboratories and education and research facilities.

SECRETARIES AT THE CENTERS

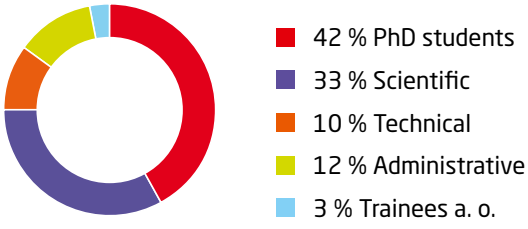
In addition to the local service units, the secretaries at the department's six centers provide general and extensive secretarial support for the center managements and scientific staff.

PRODUCTIVITY

STAFF 2011

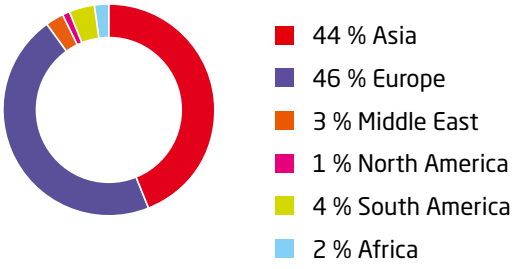
TYPE OF STAFF

(Total 243 persons)



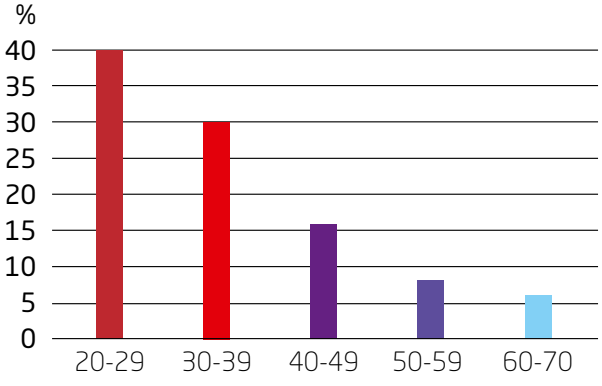
FOREIGN SCIENTIFIC STAFF

(Total 94 persons)



STAFF DISTRIBUTED BY AGE

(Total 243 persons)



PRODUCTIVITY

TEACHING & EDUCATION 2011

STUDENTS, EDUCATIONAL RESOURCES AND IMPACT

Students (STÅ*)	**189**
Completed BSc projects	**14**
Completed MSc projects	**52**

* One STÅ is the equivalent of one student studying full time in a year

RESEARCH & INNOVATION 2011

Scientific articles with referee in ISI-indexed journals (WoS)	**142**
Scientific articles with referee (non-WoS)	**4**
Contributions to refereed conference proceedings (and book series)	**25**
Monographs	**2**
Contributions to books	**20**
Dr. Thesis	**1**
PhD Theses	**27**
Scientific publications and conference contributions with no peer-review	**169**
Contribution indicated as popular	**1**
Scientific reports	**5**

PUBLICATIONS

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Jankova Atanasova, Katja; Daugaard, Anders Egede; Stribeck, Norbert; Zeinolebadi, Ahmad; Sari, Morteza Ganjaee; Potarniche, Catalina-Gabriela; Jensen, Erik Appel; Christiansen, Jesper de Claville; Hvilsted, Søren **Functional block copolymers as compatibilizers for nanoclays in polypropylene nanocomposites**. Presented at: Nordic Polymer Days. Stockholm, Sweden, 2011

Javakhishvili, Irakli; Jankova Atanasova, Katja; Tanaka, Masaru; Hvilsted, Søren **Novel block, graft and random copolymers for biomedical applications**. Presented at: Nordic Polymer Days. Stockholm, Sweden, 2011

Jonsson, Gunnar Eigil; Prado Rubio, Oscar Andres **Modeling and operation of dynamic membrane processes**. Presented at: International Congress on Membranes and Membrane Processes. Amsterdam, 2011

Kontogeorgis, Georgios; Economou, Ioannis, G.; Coutsikos, Philippos; **On the true value of cubic equations of state**, (Oral presentation), Thermodynamics 2011, Athens, Greece, 2011

Kontogeorgis, Georgios; Tsivintzelis, Ioannis; Riaz, Muhammad; Michelsen, Michael, L.; Stenby, Erling H.; **Recent applications of the CPA Equation of State for the petroleum industry**, (Poster presentation), SAFT2011, Pau, France, 2011

Kontogeorgis, Georgios; Tsivintzelis, Ioannis; Stenby, Erling H.; **Chemicals in Gas Processing (CHIGP): An industrial project for the thermodynamics of complex petroleum fluids and chemicals**, (Oral presentation), 19th European Conference on Thermophysical Properties, Thessaloniki, Greece, 2011

Lencastre Fernandes, Rita; Carlquist, Magnus; Lundin, Luisa; Heins, Anna-Lena; Dutta, Abhishek; Nopens, Ingmar; Jensen, Anker Degn; Johansen, Søren J.; Eliasson Lantz, Anna; Gernaey, Krist **Heterogeneous microbial populations: Using flow cytometric data for building dynamic distributed models**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Lencastre Fernandes, Rita; Carlquist, M.; Lundin, L.; Heins, Anna-Lena; Dutta, Abhishek; Nopens, I.; Sørensen, Søren J.; Jensen, Anker Degn; Eliasson Lantz, Anna; Gernaey, Krist **Heterogeneous microbial populations: Using flow cytometric data for building dynamic distributed models**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Lima Ramos, Joana; Tufvesson, Pär; Woodley, John **Process considerations and economic evaluation of biocatalytic production of chiral amines using transaminases**. Presented at: 8th European Congress of Chemical Engineering. Berlin, Germany, 2011

Lutze, Philip; Woodley, John; Gani, Rafiqul **A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes**. Presented at: Process Intensification Network (PIN) NL Spring Session. Utrecht, Netherlands, 2011

Lutze, Philip; Babi, Deenesh Kavi; Woodley, John; Gani, Rafiqul **Achieving process intensification: A phenomena-based synthesis/design methodology**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Lutze, Philip; Gani, Rafiqul; Woodley, John **Application of a synthesis and design methodology to achieve process intensification**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Lutze, Philip; Gani, Rafiqul; Woodley, John **Phenomena-based process synthesis and design to achieve process intensification**. Presented at: 21st European Symposium on Computer Aided Process Engineering. Chalkidiki, 2011

Lutze, Philip; Gani, Rafiqul; Woodley, John **Phenomena-based process synthesis and design to achieve process intensification**. Presented at: AIChE Spring Meeting. Chicago, USA, 2011

Mauricio Iglesias, Miguel; Johansen, Kristoffer; Jørgensen, Sten Bay; Sin, Gürkan **A Systematic methodology for the assessment and troubleshooting of control strategies and operational problems in distillation systems**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Mauricio Iglesias, Miguel; Johansen, Kristoffer; Jørgensen, Sten Bay; Sin, Gürkan **Modelling and control of heat-integrated distillation columns: An industrial case study**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen , Kaj; **An electrolyte CPA equation of state for applications in the oil and gas industry**, (Poster presentation), the 25th European Symposium of Applied Thermodynamics (ESAT), St. Petersburg, Russia, 2011

Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen, Kaj; **An electrolyte CPA equation of state for applications in the oil and gas industry,** (Poster presentation), the SAFT 2011 Workshop, Pau, France, 2011

Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen , Kaj; **Development of a CAPE-OPEN compatible library for thermodynamic models and unit operations using .NET**, (Oral presentation), the 8th European Congress of Chemical Engineering, Berlin, Germany, 2011

Meisler, Kresten Troelstrup; Abdul Samad, Noor Asma Fazli; Gernaey, Krist; von Solms, Nicolas; Gani, Rafiqul **Generic model and data based framework for analysis and development of crystallization processes**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Mitrofanov, Igor; Conte, Elisa; Abildskov, Jens; Sin, Gürkan; Gani, Rafiqul **Computer aided solvent selection and design framework**. Presented at: AIChE Annual Meeting. Minneapolis, Minnesota, USA, 2011

Mitrofanov, Igor; Sin, Gürkan; Gani, Rafiqul **Computer-aided solvent selection framework**. Presented at: CAPE forum-2011. Bradford, UK, 2011

Morales Rodriguez, Ricardo; Meyer, Anne S.; Gernaey, Krist; Sin, Gürkan **A framework for model-based optimization of bioprocesses under uncertainty: Identifying critical parameters and operating variables**. Presented at: 21th European Symposium on Computer Aided Process Engineering. Chalkidiki, Greece, 2011

Morales Rodriguez, Ricardo; Mauricio Iglesias, Miguel; Meyer, Anne S.; Gernaey, Krist; Sin, Gürkan **A framework for optimization of bioprocess operation under uncertainties: A lignocellulosic ethanol production case study**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Morales Rodriguez, Ricardo; Meyer, Anne S.; Gernaey, Krist; Sin, Gürkan **An integral analysis for second generation bioethanol production via a dynamic model-based simulation approach: stochastic nonlinear optimisation**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Morales Rodriguez, Ricardo; Meyer, Anne S.; Gernaey, Krist; Sin, Gürkan **Modelling framework for the identification of critical variables and parameters under uncertainty in the bioethanol production from lignocellulose**. Presented at: AMIDIQ XXXII National Meeting and 1st International Congress. Riviera Maya, Mexico, 2011

Morales Rodriguez, Ricardo; Meyer, Anne S.; Gernaey, Krist; Sin, Gürkan **Technology evaluation of process configurations for second generation bioethanol production using dynamic model-based simulations**. Presented at: AMIDIQ XXXII National Meeting and 1st International Congress. Riviera Maya, Mexico, 2011

Morales Rodriguez, Ricardo; Tsai, Chien-Tai; Meyer, Anne S.; Gernaey, Krist; Sin, Gürkan **Validation of inhibition effect in the cellulose hydrolysis: a dynamic modelling approach**. Presented at: AMIDIQ XXXII National Meeting and 1st International Congress. Riviera Maya, Mexico, 2011

Mortier, S.T.F.C.; Vedantam, S.; De Beer, T.; Gernaey, Krist; Remon, J.P.; Vervaet, C.; Nopens, I. **Modelling of drying processes of pharmaceutical granules. Pharmaceutical sciences for the future of medicines**. Presented at: PharmSciFair Conference. Prague, 2011

Musko, N.E.; Kontogeorgis, G.M.; Grunwaldt, J.-D.; Tsivintzelis I.; **Phase behaviour modelling of chemical reactions in dense and supercritical carbon dioxide using the cubic-plus-association equation of state**, (Poster presentation), The 25th European Symposium of Applied Thermodynamics, Saint Petersburg, Russia, 2011

Mustaffa, Azizul Azri; Díaz Tovar, Carlos Axel; Hukkerikar, Amol; Quaglia, Alberto; Sin, Gürkan; Kontogeorgis, Georgios; Sarup, Bent; Gani, Rafiqul **Building a multilevel modeling network for lipid processing systems**. *2011, Proceedings of 4th International Conference on Modeling, Simulation and Applied Optimization (ICMSAO 2011), 1-7.*

Mustaffa, Azizul Azri; Gani, Rafiqul; Kang, Jeong Won **Development and analysis of original UNIFAC-CI and modified (Dortmund) UNIFAC-CI models for predictions of VLE and SLE systems**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Nawaz, Muhammad; Zondervan, Edwin; Woodley, John; Gani, Rafiqul **Design of an optimal biorefinery**. Presented at: 21th European Symposium on Computer Aided Process Engineering. Chalkidiki, Greece, 2011

Nielsen, Mads Møller; Dimitrov, Ivaylo; Takamuku, Shogo; Jannasch, Patric; Jankova Atanasova, Katja; Hvilsted, Søren **A principal route for modification of PSU intended for PEMs by "click" chemistry**. Presented at: 2nd

PUBLICATIONS CONTINUED

International Symposium - Frontiers in Polymer Science. Lyon, France, 2011

Nielsen, Mads Møller; Dimitrov, Ivaylo; Takamuku, Shogo; Jannasch, Patric; Jankova Atanasova, Katja; Hvilsted, Søren **Conceptual structures of proton conducting polysulfone by ATRP and "click"**. Presented at: Nordic Polymer Days. Stockholm, 2011

Nielsen, Mads Møller; Dimitrov, Ivaylo; Takamuku, Shogo; Jannasch, Patric; Jankova Atanasova, Katja; Hvilsted, Søren **Modification of polysulfone for proton exchange membranes**. Presented at: EPF 5th summer school: Fundamentals and Developments in Polymer Processing Science and Technology. Gargnano, Italy, 2011

Nielsen, Mads Møller; Dimitrov, Ivaylo; Takamuku, Shogo; Jannasch, Patric; Jankova Atanasova, Katja; Hvilsted, Søren **Sulfonic acid functionalized polysulfone by "click" chemistry**. Presented at: Advances in Materials for Proton Exchange Membrane Fuel Cell Systems. Pacific Grove, CA, USA, 2011

Panchal, Chandrakant B.; Prindle, John C.; Huang, Jing; Lyczkowski, Robert W.; Doctor, Richard D.; Dada, Emmanuel A.; Lutze, Philip; Gani, Rafiqul; Woodley, John **Heat-integrated reactive distillation**. Presented at: AIChE Spring Meeting. Chicago, USA, 2011 *AIChE Spring Meeting*

Pathi, Sharat Kumar; Andersen, Maria Friberg; Lin, Weigang; Illerup, Jytte Boll; Dam-Johansen, Kim; Hjuler, Klaus **Carbonate looping for decarbonization of cement plants**. Presented at: 13. International Congress on the Chemistry of Cement. Madrid, 2011 *13. ICCC*

Perozziello, Gerardo; Møllenbach, Jacob; Laursen, Steen; Fabrizio, Enzo di; Gernaey, Krist; Krühne, Ulrich **Lab on a chip automates in vitro cell culturing**. Presented at: 37th International Conference on Micro and Nano Engineering. Berlin, 2011

Piccolo, Chiara; Piccione, Patrick M.; Gani, Rafiqul **Modeling and design of reacting systems with phase transfer catalysis**. Presented at: 21st European Symposium on Computer Aided Process Engineering. Chalkidiki, Greece, 2011

Piccolo, Chiara; Hodges, George; Piccione, Patrick M; Gani, Rafiqul **Modelling and design of phase transfer catalytic processes**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Piccolo, Chiara; Piccone, Patrick M.; Shaw, Andrew; Hodges, George; Gani, Rafiqul **Systematic computation of phase partition and solubilities in phase transfer catalytic processes**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Prado Rubio, Oscar Andres; Jørgensen, Sten Bay; Jonsson, Gunnar Eigil **Model based design and operation of a membrane bioreactor for lactic acid production**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Prado Rubio, Oscar Andres; Jørgensen, Sten Bay; Jonsson, Gunnar Eigil **Systematic procedure for integrated process operation: Reverse electro-enhanced dialysis (REED) during lactic acid fermentation**. Presented at: 21th European Symposium on Computer Aided Process Engineering. Chalkidiki, 2011

Quaglia, Alberto; Sarup, Bent; Sin, Gürkan; Gani, Rafiqul **A systematic framework for CAFD and resources allocation optimisation using MINLP in vegetable oil processing**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Quaglia, Alberto; Sarup, Bent; Sin, Gürkan; Gani, Rafiqul **Computer aided flowsheet synthesis and design under uncertainty in vegetable oil production**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Ramin, Elham; Sin, Gürkan; Mikkelsen, Peter Steen; Plósz, Benedek **Significance of uncertainties derived from settling tank model structure and parameters on predicting WWTP performance - A global sensitivity analysis study**. Watermatex. San Sebastian, Spain, 2011 *8th IWA Symposium on Systems Analysis and Integrated Assessment, 476-483*

Riaz, Muhammad; Kontogeorgis, G.M.; Stenby, E.H.; Yan, W.; Haugum, T.; Christensen, K.O.; Solbraa, E.; Løkken, T.V.; **Distribution of gas hydrate inhibitors in oil and gas production systems**, (Oral presentation), 25th European Symposium on Applied Thermodynamics, ESAT 2011, Saint Petersburg, Russia, 2011

Roughton, Brock; Camarda, Kyle V.; Gani, Rafiqul **Simultaneous design of ionic liquids and azeotropic separation for systems containing water**. Presented at: 21th European Symposium on Computer Aided Process Engineering. Chalkidiki, Greece, 2011

Roughton, Brock C.; White, John; Gani, Rafiqul; Camarda, Kyle V. **Optimal design of ionic liquid entrainers for extractive distillation of azeotrope systems**. Presented at: AIChE Annual Meeting. Minneapolis, USA, 2011

Sadegh, Negar; Kontogeorgis, Georgios; Stenby, Erling Halfdan; Thomsen, Kaj; **Thermodynamic modeling of sour gas cleaning process with alkanolamine**, (Oral presentation), 25th European symposium on Applied Thermodynamics, ESAT 2011, Saint Petersburg, Russia

Sandersen, Sara Bülow; von Solms, Nicolas; Stenby, Erling Halfdan **Phase behavior in EOR surfactant flooding**. Presented at: Thermodynamics 2011. Athens, Greece, 2011

Sandersen, Sara Bülow; von Solms, Nicolas; Stenby, Erling Halfdan **Pressure effect on phase behavior of surfactant system**. Presented at: 25th European Symposium on Applied Thermodynamics. Saint Petersburg, Russia, 2011

Sansonetti, Sascha; Conte, Elisa; Mustaffa, Azizul Azri; Crafts, Peter A.; Gani, Rafiqul **Verification and prediction of solubilities of active (pharmaceutical) ingredients in solvents and solvent mixtures**. Presented at: AIChE Annual Meeting. Minneapolis, MN, USA, 2011 *AICHE American Congress of Chemical Engineering*

Sengeløv, Louise With; Thomsen, Kaj **Phase equilibrium in amino acid salt systems for CO_2 capture**. Presented at: WORKSHOP - Amino Acid Salts for CO_2 Capture. Adminiet, Porsgrunn, Norway, 2011

Sin, Gürkan; Gani, Rafiqul **Model-based engineering for product-process design - dealing with uncertainties** *Chemical Engineering Greetings to Prof. Sauro Pierucci: on occasion of his 65th birthday, 277-286*

Singh, Ravendra; Rozada-Sanchez, Raquel; Wrate, Tim; Muller, Frans; Gernaey, Krist; Gani, Rafiqul; Woodley, John **A retrofit strategy to achieve "Fast, Flexible, Future (F3)" pharmaceutical production processes**. Presented at: 21th European Symposium on Computer Aided Process Engineering. Chalkidiki, Greece, 2011

Singh, Ravendra; Rozada-Sanchez, Raquel; Wrate, Tim; Muller, frans; Gernaey, Krist; Gani, Rafiqul; Woodley, John **Substrates adoption methodology (SAM) to achieve "Fast, Flexible, Future (F3)" pharmaceutical production processes**. Presented at: 8th European Congress of Chemical Engineering. Berlin, 2011

Skov, Anne Ladegaard; Bejenariu, Anca Gabriela; Daugaard, Anders Egede **Influence of micro- and nanofillers on DEAP performance**. Presented at: World Congress on Biomimetics, Artificial Muscles and Nano-Bio. Paris, France, 2011

Skov, Anne Ladegaard; Kiil, Søren **Teaching chemical product design to engineering students: course contents and challenges**. Presented at: 7th International CDIO Conference. Technical University of Denmark, Kgs. Lyngby, 2011

Smets, Barth F.; Mutlu, A. Gizem; Pellicer i Nàcher, Carles; Jensen, Marlene Mark; Vangsgaard, Anna Katrine; Sin, Gürkan; Gernaey, Krist; Vlaeminck, Siegfried **Micro2-managed microbial communities: Next generation environmental bio/technologies**. Presented at: 1st International Symposium on Microbial resource management in biotechnology: Concepts & Applications. Ghent, Belgium, 2011

Szabo, Peter; Clasen, Christian; McKinley, Gareth H. (2011): **Constant force extension in polymer solutions: Extended abstract of paper**. Presented at: 20th Nordic Rheology Conference. Helsinki, 2011 *Nordic Rheology Society. Annual Transactions, 19*

Thomsen, Kaj **Current status of R&D in post combustion CO_2 capture**. Presented at: CHALMERS ENERGY CONFERENCE. Gothenburg, Sweden, 2011

Thomsen, Kaj **Phase equilibrium in amino acid salt systems for CO_2 capture**. (Invited speaker) at Gassonova, Norway, 2011

Thomsen, Kaj **Chemical absorption materials for CO_2 capture**. (Invited speaker) at ICEPE2, Second International Conference on Energy Process Engineering, DECHEMA-Haus, Frankfurt am Main, Germany, 2011

Tsivintzelis, Ioannis; Beier, Matthias; Grunwaldt, Jan-Dierk; Kontogeorgis, Georgios M.; **Phase equilibria of mixtures related to the catalytic oxidation of alcohols in supercritical CO_2: An experimental and theoretical study,** (Poster presentation), the19th European conference on Thermophysical Properties (19th ECTP), Thessaloniki, Greece, 2011

Tsivintzelis, I.; Kontogeorgis, G.M.; Michelsen, M.; Stenby, E.H.; **Modeling of mixtures with acid gases using the CPA equation of state**, (Poster presention), The 25th European Symposium of Applied Thermodynamics, Saint Petersburg, Russia, 2011

Tsivintzelis, Ioannis; Kontogeorgis, G. M.; **On the complex hydrogen bonding behavior of organic acids**, (Oral presentation), *Proceedings og the 8th Hellenic Conference of Chemical Engineering Electronic verion,Thessaloniki, Greece, 2011*

Tsivintzelis, Ioannis; Michelsen, Michael L.; Stenby, Erling H.; Kontogeorgis, Georgios M.; **Modeling of mixtures with acid gases using CPA,** (Poster presentation) *Proceedings of Thermodynamics 2011. Book of abstracts, page 428-430, Athens, Greece, 2011*

Tufvesson, Pär; Lima Ramos, Joana; Jensen, Jacob Skibsted; Woodley, John **Operating windows for transaminase processes using thermodynamic and biocatalyst constraints**. Presented at: BIOTRANS 2011. Giardini Naxos (IT), 2011 *Biotransformations in organic synthesis, 105*

Vangsgaard, Anna Katrine; Mauricio Iglesias, Miguel; Gernaey, Krist; Smets, Barth F.; Sin, Gürkan **Framework for construction of multi-scale models for biological wastewater treatment processes**. Presented at: IWA Symposium on Systems Analysis and Integrated Assessment. San Sebastian, Spain, 2011

Vergara-Fernández, A.; Rebolledo-Castro, J.; Morales Rodriguez, Ricardo **Multiscale modelling approach for a fungal biofilter unit**

PUBLICATIONS CONTINUED

for the hydrophobic abatement of volatile organic compounds. Presented at: AMIDIQ XXXII National Meeting and 1st International Congress. Riviera Maya, Mexico, 2011

Völcker, Carsten; Jørgensen, John Bagterp; Stenby, Erling Halfdan **Oil reservoir production optimization using optimal control**. *2011, Proceedings of 50th IEEE Conference on Decision and Control and European Control Conference*

Waseem Arshad, Muhammad; Thomsen, Kaj **Freezing point depression of aqueous solutions of DEEA, MAPA and DEEA-MAPA with and without CO_2 loading**. Presented at: 2nd ICEPE. Frankfurt am Main, 2011

Wu, Qiongxiao; Christensen, Jakob Munkholt; Chiarello, Gian Luca; Temel, Burcin; Grunwaldt, Jan-Dierk; Jensen, Anker Degn **Supported molybdenum carbides for higher alcohols synthesis from syngas**. 2011, Proceedings of 242nd ACS National Meeting. *American Chemical Society. Division of Fuel Chemistry. Preprints of Symposia, 55(1)*

Wu, Qiongxiao; Christensen, Jakob Munkholt; Temel, Burcin; Grunwaldt, Jan-Dierk; Jensen, Anker Degn **Supported Cu/Group VIII metal alloys for synthesis of alcoholic fuels from syngas**. Presented at: The 22nd North American Catalysis Society Meeting. Detroit, USA, 2011

Xu, Yuan; Nordblad, Mathias; Brask, Jesper; Woodley, John **Development of process technology for two-stage enzymatic FAEE-biodiesel production**. Presented at: 8th European Congress of Chemical Engineering, Berlin

Xue, Rui; Mikkelsen, Jørn Dalgaard; Meyer, Anne S.; Woodley, John **Reactor selection for multi-enzymatic processes**. Presented at: 10th International Symposium on Biocatalysis and Biotransformations. Giardini Naxos, Sicily, Italy, 2011 *10th International Symposium on Biocatalysis and Biotransformations*

Yuan, Hao; Shapiro, Alexander **Filtration in porous media: Influential parameters and comparison with experiments**. Presented at: Third International Conference on Porous Media. Bordeaux, France, 2011

Yuan, Hao; Nielsen, Sidsel Marie; Shapiro, Alexander; Stenby, Erling Halfdan **Particles and pores: New transport and capture mechanisms**. Presented at: CERE discussion meeting 2011. Pharmakon, Hillerød, 2011

Yuan, Hao; Shapiro, Alexander; Stenby, Erling Halfdan **Physical mechanisms of deep bed filtration with application to the problems of petroleum industry**. Presented at: 2011 Bit's 2nd Annual World Congress of Well Stimulation and EOR. Congqing, China, 2011

Yuan, Linfeng; Korsholm, Lars; Jakobsen, Sune; Woodley, John; Jonsson, Gunnar Eigil **Electromembrane filtration: An alternative way to fractionate industrial enzymes**. Presented at: ICOM 2011. Amsterdam, 2011

Yunus, Nor Alafiza; Gernaey, Krist; Woodley, John; Gani, Rafiqul **Design of tailor-made fuel blends of gasoline and bio-fuels**. Presented at: International Congress on Sustainability Science and Engineering. Tucson, 2011

Yunus, Nor Alafiza; Manan, Zainuddin Abd.; Gernaey, Krist; Woodley, John; Gani, Rafiqul **Tailor-made design of chemical blends using decomposition-based computer-aided approach**. Presented at: ICMSAO. Kuala Lumpur, 2011

Yan, Wei; Langlais, C.; Stenby, E.H.; **Viscosity modelling of alcohols using the CPA EoS and the friction theory**, (Poster presentation), 19th European Conference on Thermophysical Properties, 19th ECTP, Thessaloniki, Greece, 2011

Yan, W.; Michelsen, M.L., Stenby, E.H.; **Non-cubic EoS for reservoir simulations: Computation time and PVT modelling**, (Poster presentation), SPE Applied Technology Workshop Complex Reservoir Fluids—New Developments and Multi-Discipline Integration, Amsterdam, The Netherlands, 2011

Yan, W.; Michelsen, M.L.; Stenby, E.H. 2011: **On application of non-cubic EoS to compositional reservoir simulatio**n, (Oral presentation), the SPE EUROPEC/EAGE Annual Conference and Exhibition held in Vienna, Austria, SPE 142995

Yan, Wei; Michelsen, Michael L.; Stenby, Erling H.; **Two practical aspects of compositional reservoir simulations with PC-SAFT,** (Poster presentation), SAFT2011, Pau, France

Yan, W.; Michelsen, M.L.; Stenby, E.H.; Belkadi, A.; **On two flash methods for compositional reservoir simulations: Table look-up and reduced variables,** (Oral presentation), the 32nd Annual Symposium and Workshop for the IEA Collaborative Project on Enhanced Oil Recovery, Vienna, Austria, 2011

Zahid, Adeel; Sandersen, Sara Bülow; Shapiro, Alexander; von Solms, Nicolas; Stenby, Erling Halfdan; Yuan, Hao **Advanced waterflooding in chalk reservoirs: crude oil/brine interaction study**. Presented at: 2011 Bit's 2nd Annual World Congress of Well Stimulation and EOR. Congqing, China, 2011

Zeuner, Birgitte; Riisager, Anders; Meyer, Anne S. **Activity and stability of feruloyl esterase A from *Aspergillus niger* in ionic liquid systems**. Presented at: 6th Danish Conference on Biotechnology and Molecular Biology - Synthetic Biology and Cell Factories. Vejle, 2011

Contributions indicated as popular

Cervera Padrell, Albert Emili; Skovby, Tommy; Kiil, Søren; Gernaey, Krist (2011): **Kontinuerlig lægemiddelproduktion af små molekyler via organisk syntese** Dansk Kemi, 92(11), 18-20.

Scientific reports

Ahrenfeldt, Jesper; Henriksen, Ulrik Birk; Münster-Swendsen, Janus; Fink, Anders; Clausen, Lasse Røngaard; Christensen, Jakob Munkholt; Qin, Ke; Lin, Weigang; Jensen, Peter Arendt; Jensen, Anker Degn (2011): **Production of methanol/DME from biomass: EFP06** - Risø DTU, 2011 *CHEC; R1107*

Gani, Rafiqul; Woodley, John (2011): **CAPEC-PROCESS Research Report 2011** - Kgs. Lyngby: DTU Chemical Engineering, 2011

Hansen, Brian Brun; Jensen, Anker Degn; Jensen, Peter Arendt (2011): **REBECa WP IV - Formation and transformation of particles and other pollutants from engines using biofuel: WP IV final report (DTU project no. 50502)** - DTU Chemical Engineering, 2011 *CHEC; R1106*

Iyara, N.; Siemanond, K.; Gani, Rafiqul (2011): **Sustainable design for an olefin process: Internal report** - DTU Chemical Engineering, 2011

Tansutapanich, P.; Malakul, P.; Gani, Rafiqul (2011): **Sustainable process design for lignocellulosic-based bioethanol using life cycle assessment technique: Internal report** - DTU Chemical Engineering, 2011

MASTER'S AND BACHELOR COURSES

The department participates in a 3½ year education for the Bachelor of Engineering, a 3 year education for Bachelor of Science and a 2 year education for the Master of Engineering. Below, course numbers and names are shown for 2011, with the number of students attending shown in brackets. Courses for Bachelor of Engineering are marked with (**B**). The other courses are Master courses or common courses.

SPRING SEMESTER

28001 Introduction to Chemistry and Chemical Engineering (48)
28012 Chemical and Biochemical Process Engineering (32) (**B**)
28016 Mathematical models for chemical and biochemical systems (22) (**B**)
28017 Chemical and Biochemical Process Engineering (3) (**B**)
28020 Introduction to Chemical and Biochemical Engineering (71)
28022 Unit Operations of Chemical Engineering and Biotechnology (28) (**B**)
28121 Chemical Unit Operations Laboratory (6)
28122 Chemical Unit Operations Laboratory – Summer University for Europeans (7)
28157 Process Design (30) (**B**)
28160 Mathematical models for chemical systems (36)
28212 Polymer Chemistry (22)
28221 Chemical Engineering Thermodynamics (20)
28231 Laboratory in Chemical and Biochemical Engineering (16)
28322 Chemical Engineering Thermodynamics (24) (**B**)
28342 Chemical Reaction Engineering (28) (**B**)
28345 Chemical Reaction Engineering (29)
28350 Process Design: Principles and Methods (39)
28352 Chemical Process Control (25) (**B**)
28415 Oil and Gas Production (22)
28423 Phase Equilibria for Separation Processes (17)
28434 Membrane Technology (37)
28443 Industrial Reaction Engineering (34)
28451 Optimizing Plantwide Control (17)
28850 Quality by Design (QbD): Integration of product and process development (11)
28852 Risk Assessment in Chemical Industry (44)
28855 Good Manufactoring Practice (49)
28864 Introduction to Matlab Programming (25)
28885 Technology and Economy of Oil and Gas Production (21) (**B**)

Courses given in cooperation with other departments:

26316 Analysis and Chromatography (44)
27944 Biotechnology and process design (23) (**B**)
31525 Physiological transport phenomena (9)
41683 Materials Science (35) (**B**)

EDUCATION CONTINUED

MASTER'S AND BACHELOR COURSES

FALL SEMESTER

28012 Chemical and Biochemical Process Engineering (55) (**B**)
28016 Mathematical models for chemical and biochemical systems (36) (**B**)
28022 Unit Operations of Chemical Engineering and Biotechnology (32) (**B**)
28121 Chemical Unit Operations Laboratory (21)
28140 Introduction to Chemical Reaction Engineering (24)
28150 Introduction to Process Control (21)
28156 Process and product design (21) (**B**)
28213 Polymer Technology (22)
28233 Recovery and Purification of Biological Products (32)
28244 Combustion and High Temperature Process (56)
28246 Applied Enzyme Technology and Kinetics (37)
28247 Advanced Enzyme Technology (15)
28310 Chemical and Biochemical Product Design (43)
28315 Colloid and Surface Chemistry (34)
28316 Laboratory Course in Colloid and Surface Chemistry (15)
28322 Chemical Engineering Thermodynamics (31) (**B**)
28342 Chemical Reaction Engineering (35) (**B**)
28352 Chemical Process Control (29) (**B**)
28361 Chemical Engineering Model Analysis (65)
28420 Separation Processes (41)
28515 Enhanced Oil Recovery (14)
28530 Transport Processes (49)
28811 Polymers in Processes and Products (8)
28845 Chemical Reaction Engineering Laboratory (24)
28864 Introduction to Matlab Programming (38)

Courses given in cooperation with other departments:

10336 Fundamentals Problems in Fluid Dynamics (12)
12411 Introduction to Petroleum Technology (29)
23522 Rheology of food and biological materials (10)
26010 Introductory Project in Chemistry (55)
27004 Health, Diseases and Technology (47)
27944 Biotechnology and process design (24) (**B**)
41657 Materials Science for Chemists (30)
41683 Materials Science (29) (**B**)

MASTER OF SCIENCE DEGREES

52 students finished their research projects for the MSc degree. The project titles and names of the students are listed below:

Ali, Shahid
Application of the CPE EoS to CO_2 mixtures

Andersson, Louise Grann
Method Development for Evaluation of Novel Proteolytic Enzymes

Arnourgi, Eleni
Optimization and characterization of a peroxidise from Coprinopsis

Awad, Hassan
Liquid Fuel Hydro-desulphurisation for Solid Oxide Fuel Cell Application

Babi, Deenesh Kavi
Heat Transfer within a Biomass Particle During Devolatilization

Bacher, Pernille
Process development of enzymatic fish oil ethanolysis

Balduck, Guillaume Etienne Marcel
Experimental Analysis and Modelling to Identify the Mechanism and Kinetic of Cellulases

Bonnek, Peter Løvengreen
Mathematical Modelling of Municipal Waste Incineration on a Moving Grate

Calafat Frontera, Joan
Carbonate Looping Process for CO_2-Capture

Cepulyte, Daila
Enzymatic Reaction Design: Novel Saccharide Reactions

Christensen, Troels Juel
Grinding of Biomass

Chys, Michael Etienne Eliane
Yeast cultivations in Microbioreactors

Claridge, Tais Bjerg
Modelling of H2S Absorption in ZnO piller

Cortada Mut, Maria del Mar
Rain Erosion Coatings for Wind Turbines Blades

Damgaard, Pernille
Assessment of Electrostatics Involved in Polyelectrolyte Adsorption onto Surfaces via Zeta Potential Technology

Enemark-Rasmussen, Rasmus
A framework for computer-aided HAZOP studies supported by dynamic simulations

Gao, Lei
Rheology of Interpenetrating Networks

Godfroy, Pierre
Design of Sustainable Separation Processes

Gomis Cañete, Maria
Optimization of the Dispersion step in Paint Production

De Haas, Erin
Gas Diffusivity in Heavy Oil and Its Influence on Foamy Oil Behavior

Halck, Christina Steenberg
Modeling of Molecular Transport and Absorption in Surface-based Biosensors

Hansen, Troels Bruun
Combustion Characterization of Alternative Fuels

Helling, Ayelén
Physical Properties of Light-responsive Materials

Hudecz, Diana
Continuous Crystallization of an Active Pharmaceutical Ingredient

Johansen, Joakim Myung
Combustion of Biomass

Jølck, Malene Irming
Xylanase Catalysed Viscosity Reduction

Khandelwal, Ankit
Solvent Based Organic Synthesis

Lotero Herranz, Irene
Carbonate looping for CO_2 capture

Meisler, Kresten Troelstrup
Crystallization Operation Modelling

EDUCATION CONTINUED

MASTER OF SCIENCE DEGREES CONTINUED

Mikkelsen, Søren
Novel Aluminophosphates for Selective Catalytic Reduction of NOx

Mohn, Thomas Uffelmann and Hans Jerik Folmer Thøgersen
Development of Green Polymers for Gas Hydrate Inhibition

Nawaz, Muhammad
Sustainable Biorefinery Design and Analysis

Nielsen, Joachim Bachmann
Filtering of diesel exhaust gas

Nørby, Martin
Modeling and Simulation of Continuous Fluid Bed Processes

Olsen, Brian Kjærgaard
Kinetics of Adiabatic Reforming

Pedersen, Michael Jønch
Progress in the Novel Development of Continuous Process Design for Modern Pharmaceutical Production

Pereira Rosinha, Ines
High frequency backshock effect on ultrafiltration of selected polysaccharides

Price, Jason Anthony
Regression of parameters in dynamic kinetic models

Ramesh, Hemalata
Continuous enzymatic production of alkyl esters in a multi-phasic reaction system

Ravn, Helle Christine
Optimization of Reaction Parameters for Enzymatic Triglyceride Synthesis from Fish Oil Ethyl Esters and free Fatty Acids

Rey. Charlotte Elisée Eugénie
Assessment of production profiles for Shale Gas reservoirs

Ringborg, Rolf Hoffmeyer
Optimizing the preparation of zeozymes

Rueda, Miriam and Ruth Solá
Oil/water Emulsions in Oil Reservoirs

Serrano Briega, Guillermo
Evaluation of coupled dehydrogenase systems

Stasiukélyté, Migle
Understanding Adhesion of Silicone Based Tiecoats to Epoxy Substrates

Stokelj, Tina
New enzymatic starch degradation strategies in brewing

Weiss, Noah Daniel
Evaluation of Enzyme Re-use in Lignocellulose Processing

Xue, Rui
Enzymatic Production of Biodiesel: Reaction Engineering

Yussuf, Mustafe Ahmed
Measurement of Phase Equilibria for Oil-Water-MEG Mixtures

Zhang, Dong
Software development for model-based upscaling of fermentation processes

BACHELOR OF SCIENCE IN ENGINEERING DEGREES

9 students finished their research program for the BSc degree. The project titles and names of the students are listed below:

Ali Akbari Sefid Darbony, Ahmad Reza
Chemical and Hydrothermal Stability of Ammonia Slip Catalysts

Andersen, Søren Henckel
Investigation and modelling of novel pre-heating process for application in cement production

Christoffersen, Ann-Louise Nygård
In-line determination of structure in precipitation processes

Eeg, Tina Drejer
Removal of Amino Acids from Orange Juice

Jespersen, Steffen Ehlerts
Stability of Alternative Tile Materials

Mortensen, Asmus Ringlebjerg
Moving from Batch Towards Continuous Organic-chemical Pharmaceutical Production

Munk, Thomas
Ash Deposit Formation in Biomass-Fired Boilers

Roed, Anders
CCSEM analysis of clinker products

Sørensen, Kim
Energy Efficiency in an Oil Refinery – Air Preheater Design and Investigation of Waste-heat Recovery

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ADVISORY BOARD

LARS BANG

VICE PRESIDENT · H. LUNDBECK A/S

Scientific research at university level is a prerequisite for the development of Lundbeck's chemical activities in Denmark. We have had a beneficial cooperation with DTU Chemical Engineering for several years, collaborating on PhD projects and recruiting several of its candidates. Furthermore, it has been a great advantage to be able to draw on the knowledge of DTU Chemical Engineering's scientific staff as advisors/consultants.

KIM PANDRUP CHRISTENSEN

VICE PRESIDENT · ANDRITZ FEED & BIOFUEL A/S

The close cooperation with DTU Chemical Engineering will ensure significant results within the biofuel technology which will benefit a lot of industries. Long-term focus on development and innovation is necessary to meet the ever changing opportunities, rules and legislation that most industries will have to comply with. DTU Chemical Engineering ensures a high level of education and important research projects that will lead to technologies of the future.

PER FALHOLT

EXECUTIVE VICE PRESIDENT · NOVOZYMES A/S

In terms of industrial collaboration DTU Chemical Engineering is at the front-line and our cooperation is exemplary. For Novozymes it is very important that possible future technologies are developed and tested within a university framework where new valuable employees get their education and where real solutions to major challenges to society are found. DTU Chemical Engineering fully answers these demands, benefiting both society and Novozymes.

BJERNE CLAUSEN

CEO · HALDOR TOPSØE A/S

Working closely with the best research groups within the fields of our core competences is of major importance to Haldor Topsoe A/S. Our cooperation with DTU Chemical Engineering enables us to resolve research challenges beyond our competences and resources and is an important source of inspiration and knowledge for employees at Haldor Topsoe, benefiting their own and the company's development.

Welcome to Executive Vice President Peder Holk Nielsen who joins the Advisory Board in 2012.

PEDER HOLK NIELSEN

EXECUTIVE VICE PRESIDENT · ENZYME BUSINESS · NOVOZYMES A/S

STUDENT COMMITTEE

KTStudents is the student organization at DTU Chemical Engineering. KT-Students seek to provide engineering and non-engineering related activities for students that are part of or affiliated with the department. These activities span over a wide range and include:

1. **Company and Technical Presentations** – companies are invited to present an overview of their work and a technical lecture so the attending students have an idea of the type of R&D or engineering tasks faced at the company

2. **Company Trips** – company sites are visited by the students. These events are normally fully funded by the companies themselves and the companies typically have production or pilot facilities which give students an image of the real world

3. **Social Events** – The goal of these are to give students the opportunity to socialize and net-work with other students whom they would otherwise be unable to meet during the hectic semester

4. **Research Opportunities** – This has been held by KTStudents for the past two years. The 6 research centers at the department present research opportunities at their centers ranging from BSc over MSc to PhD projects

5. **Roundtable discussions** – This has been held jointly with the department the last two semesters. When a leading researcher visits the department, the students have an exclusive opportunity to meet the researcher and discuss a wide range of topics

In November 2010, KTStudents became the 1st student chapter in Europe to house an American Institute of Chemical Engineers (AIChE) Student Chapter. The AIChE is the largest society for chemical engineers, offering technical information and networking for studying and practicing chemical engineers.

KTStudents continues to expand with an ambitious plan in 2012 to hold our first annual one-day student conference where students from the BSc and MSc levels will have the opportunity to present their research and projects at oral and poster sessions.

Asbjørn Toftgaard Pedersen, President, KTStudents

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DEPARTMENTAL SEMINARS AT DTU CHEMICAL ENGINEERING IN 2011

FEBRUARY 10

Louise Olsson, Chalmers University of Technology, Sweden

"Emission cleaning from vehicles using heterogeneous catalysis"

MARCH 23

Professor Sigurd Skogestad, Norwegian University of Science and Technology, Norway

"A systematic approach to plantwide control"

MAY 3

Professor Jean-Noël Jaubert, University of Nancy, France

"Towards a group-contribution method to predict temperature-dependent binary interaction parameters (kij) whatever the cubic equation of state and the associated alpha function"

SEPTEMBER 8

Professor Richard Darton, University of Oxford, UK

"Measuring sustainability with indicator sets"

OCTOBER 4

Professor, Dr. Michael R. Buchmeiser, University of Stuttgart, Germany

"Monolithic Polymeric Supports for Separation Science, Heterogeneous Catalysis and Tissue Engineering"

NOVEMBER 15

Professor E.L. Cussler, University of Minnesota, USA:

"A Different Chemical Industry"

USEFUL INFORMATION

Guide to the department

- Department of Chemical and Biochemical Engineering
- Administration, offices, DTU cafeterias, Student House
- Departments/centers
- Auditoriums
- Oticon Hall
- Halls of residence/shared facilities
- SCION.DTU
- Physical Plant
- Parking
- Bus stop

This Annual Report 2011 may be ordered
from the reception at the Department of
Chemical and Biochemical Engineering, DTU.

Also available on www. kt.dtu.dk

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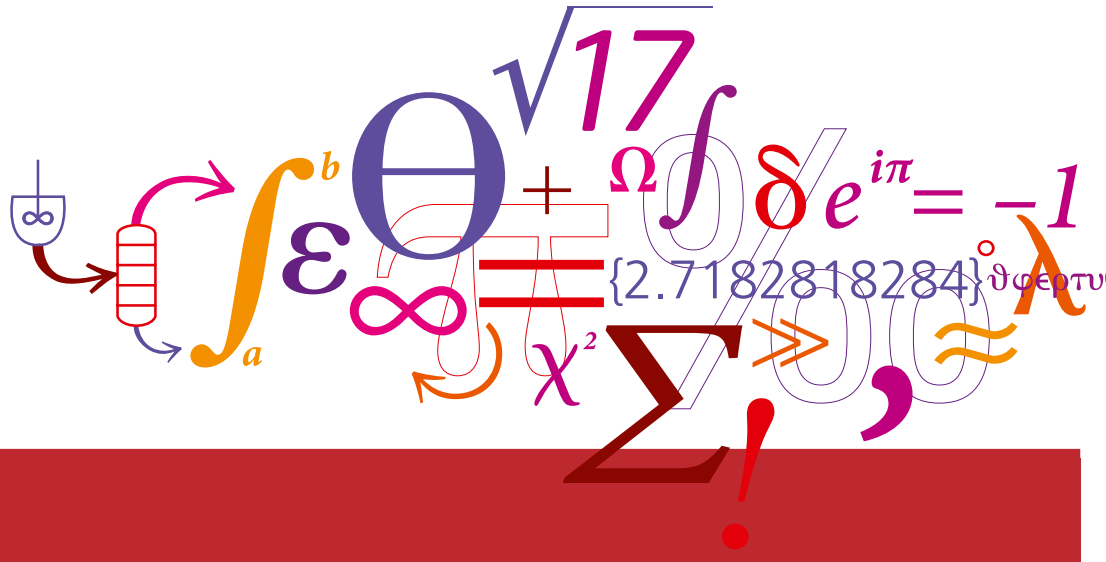
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